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Moment methods with effective nuclear Hamiltonians: calculation of radial moments

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MOMENT METHODS WITH EFFECTIVE NUCLEAR HAMILTONIANS; CALCULATION OF RADIAL MOMENTS

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Moment methods with effective nuclear Hamiltonians; calculation of radial moments

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I. INTRODUCTION

In this work we will use the average diagonal matrix elements of many-body operators (1) averaged over shell model states with no core (2) in order to solve nuclear many-body problems. Since these operator averages, called moments, are invariant under unitary transformations we may calculate them in the simpler shell model basis.

Specifically, we will use these moment methods to calculate the ground state expectation value of the radial moments of the one-body density. The ground state is described by an effective nuclear Hamiltonian (2). We will use a truncated expansion in terms of the orthogonal polynomials of the eigenvalue distribution of the Hamiltonian.

In Chapter II we discuss the principles of shell model spaces and define the effective nuclear Hamiltonian. Included is a discussion of the creation and destruction operator representation which is used in the formulation for the moments of many-body operators.

In Chapter III we define scalar, as well as configuration, moments of many-body operators and discuss trace invariance under unitary transformations. We discuss the trace reduction formulae (3,4) and we present some of the simpler cases in detail. Finally, we discuss the orthogonal polynomial expansion for the expectation value of a general many-body operator.

In Chapter IV we apply the theory discussed in the previous two chapters in order to express the formula for the expectation values at the radial moments. Included is a discussion of the use of configuration

moments to calculate radial moment expectation values for states with good total isospin.

In the last chapter we evaluate the lower radial moment expectation values for the nuclei ^{16}O, ^{40}Ca, and ^{58}Ni, compare the results with other theoretical predictions, and discuss the effects of the model space size and effective interaction parameters. Finally, with a method that employs radial moment expectation values in the calculation of elastic electron scattering cross sections, we test the radial moment expectation values with experimental data and show that good agreement can be obtained.

II. SHELL MODEL ESSENTIALS AND INTERACTIONS

In this chapter, in Section A, we will discuss the nuclear shell model basis in terms of which the theory will be cast. In Section B we will write the Hamiltonian and basis vectors in terms of fermion creation and destruction operators. In Section C we discuss the nucleon-nucleon interaction that is used in this work. In Section D we define the effective Hamiltonian which is valid for working in a finite shell model space, and in Section E we discuss a phenomenological effective interaction, the Kallio-Koltveit interaction.

A. Shell Model and the Pauli Principle

Let H be the Hamiltonian of an m-nucleon system, where each particle is subject to one and two body forces, that is

$$H = O + V \tag{2.1}$$

where

$$O = \sum_{i=1}^{m} o(i) \tag{2.2}$$

and

$$V = \frac{1}{2} \sum_{\substack{i,j=1 \\ i \neq j}}^{m} v(i,j) \quad . \tag{2.3}$$

It should be mentioned that although the importance of three and four body interactions is not completely clear, recent work (5) has shown that these interactions may be significant, at least for light nuclei.

In this work, however, we will restrict the Hamiltonian form to one and two body terms.

The solutions to the Schroedinger equation

$$H|B\rangle = E_B|B\rangle \quad , \quad B = 1, \ldots, \infty \tag{2.4}$$

are the m-particle state vectors $|B\rangle$ with energy E_B. Also, the states are ordered so that $E_1 \leq E_2 \leq \ldots$. Since H is taken to be a Hermitian operator, its eigenvectors can be chosen mutually orthogonal. If we then normalize each eigenvector to unity, we can write

$$\langle B|C\rangle = \delta_{BC} \quad , \quad B,C = 1, \ldots, \infty \quad . \tag{2.5}$$

The Schroedinger equation for a m-body Hamiltonian H_o which is the sum of one-body Hamiltonians h(i) is easily solved for both eigenvectors and energies so that the m-particle vector basis, referred to as the shell model basis, is a convenient one in which to pose many body calculations. The shell model Hamiltonian is

$$H_o = \sum_{i=1}^{m} h(i) = \sum_{i=1}^{m} (t(i) + u(i)) \tag{2.6}$$

where t(i) is the kinetic energy of the i-th particle and u(i) is the one-body potential. The one-body Schroedinger equation is

$$h(i)|\alpha(i)\rangle = \varepsilon_\alpha|\alpha(i)\rangle \quad , \quad \alpha = 1, \ldots, \infty \tag{2.7}$$

where the eigenvector $|\alpha(i)\rangle$ of the i-th particle has an eigenenergy ε_i and quantum state labels, including spin and isospin, are represented by (i). Some scheme can be used to place the state label α in one-to-one correspondence with the quantum numbers of the unique state.

One choice for h, using self-consistent techniques (6), would give H_o certain averaged properties of H. However, this is difficult to perform, so for convenience we will take the usual choice of a spherical harmonic oscillator potential (7) for h. For this case $\alpha \leftrightarrow (n_\alpha, \ell_\alpha, j_\alpha, m_\alpha, t_{z\alpha})$, where n_α is the principal quantum number for the orbit, ℓ_α represents the orbital angular momentum, j_α represents the total angular momentum (orbital plus spin), m_α is the total angular momentum projection, and $t_{z\alpha}$ is the isospin projection. Also, the eigenenergies are

$$\varepsilon_\alpha = (2n_\alpha + \ell_\alpha + 3/2)\hbar\Omega \quad ,$$

where $\hbar\Omega$ is known as the oscillator constant and specifies the spacing between shells.

The Schroedinger equation for the shell model Hamiltonian is

$$H_o|\Gamma\rangle = E_\Gamma|\Gamma\rangle \quad , \quad \Gamma = 1, \ldots, \infty \quad . \tag{2.8}$$

The state labeled Γ specifies the m harmonic oscillator states (α, β, ..., η) occupied by the m noninteracting particles.

Because we are dealing with a system of identical fermions, the Pauli principle requires that each m-particle state vector be antisymmetric under the exchange of any two particle labels. This requirement is incorporated in the shell model basis by writing $|\Gamma\rangle$ as a Slater determinant of the single particle states, i.e.

$$|\Gamma\rangle = \frac{1}{\sqrt{m!}} \begin{vmatrix} |\alpha(1)\rangle & |\beta(1)\rangle & \cdots & |\eta(1)\rangle \\ \vdots & & & \\ |\alpha(m)\rangle & |\beta(m)\rangle & \cdots & |\eta(m)\rangle \end{vmatrix} . \qquad (2.9)$$

Note that because of this antisymmetric property of the m-particle states, m! linearly dependent vectors can be constructed for each set of m occupied single particle orbitals. Because we want a linearly independent shell model basis, we must choose a unique ordering of the single particle labels for each set when we define our basis states.

For a sum of one-body Hamiltonians, the total energy of a given state is the sum of the energies of the occupied single particle states,

$$E_\Gamma = \varepsilon_\alpha + \varepsilon_\beta + \cdots + \varepsilon_\eta \quad .$$

Because of the last equality, if degeneracies exist among two or more single particle states (true for the spherical harmonic oscillator) then degeneracies may exist among the m-particle shell model states.

Making an expansion of the eigenbasis of H in terms of the shell model basis,

$$|B\rangle = \sum_{\Gamma=1}^{\infty} D_{B\Gamma} |\Gamma\rangle \quad , \qquad B = 1, \ldots, \infty \quad , \qquad (2.10)$$

and operating on the expansion with a conjugate expansion gives

$$\langle C|B\rangle = \sum_{\Gamma,\Lambda=1}^{\infty} D^*_{C\Lambda} D_{B\Gamma} \langle\Lambda|\Gamma\rangle \quad .$$

Since (2.5) holds for the eigenvectors of any Hermitian operator, the

last equation becomes

$$\delta_{CB} = \sum_{\Gamma=1}^{\infty} D^{*}_{C\Gamma} D_{B\Gamma} \quad , \tag{2.11}$$

which is the definition of a unitary transformation. That is, the states of the full Hamiltonian are related to shell model states by a unitary transformation.

B. Operator Representation

Here we discuss the operator representation for the state vectors and interactions. The operator representation is also known as the formalism of second quantization and is much more convenient for operator manipulation, especially with the utilization of Wick's theorem (Appendix A).

We will begin by defining $|0\rangle$ as the state vector for the "vacuum" or reference state. This state is often taken to be noninteracting core. We take $\langle 0|0\rangle = 1$. Next we introduce the creation operator, a_α, which creates a particle in the single particle state α when it acts on the vacuum, i.e.,

$$a_\alpha|0\rangle = |\alpha\rangle \quad , \tag{2.12}$$

where $|\alpha\rangle$ is the vector denoting the occupied state α. Similarly, we define a destruction operator, b_α, which destroys a particle in state α when it acts on $|\alpha\rangle$, i.e.,

$$b_\alpha|\alpha\rangle = |0\rangle \quad , \tag{2.13}$$

and gives zero when it operates on the vacuum, or on a vector with state label different from α, i.e.,

$$b_\alpha|0\rangle = 0 \quad \text{and} \quad b_\alpha|\beta\rangle = 0 \quad , \quad \text{if } \alpha \neq \beta \quad . \tag{2.14}$$

The adjoint of (2.12) is

$$\langle 0|a_\alpha^+ = \langle\alpha| \quad .$$

With the requirement that the single particle wave vectors be orthonormal, $\langle\alpha|\beta\rangle = \delta_{\alpha\beta}$, we can operate on (2.14) with the vector $|\alpha\rangle$ giving

$$\langle 0|a_\alpha^+|\alpha\rangle = 1 \quad .$$

If a_α^+ is interpreted as acting on $|\alpha\rangle$ rather than $\langle 0|$, then it must be true that

$$a_\alpha^+|\alpha\rangle = |0\rangle \quad ,$$

if the vacuum is taken to be normalized. Thus

$$b_\alpha \equiv a_\alpha^+ \quad , \tag{2.15}$$

which means that b_α is a particle destruction operator when it acts to the right and a creation operator when it acts to the left, that is, when acting as the adjoint operator. A similar argument can be used to show that a_α is a destruction operator when it acts to the left as well as a creation operator when acting to the right.

The utility of the operator representation is seen in its ability to transform between spaces with different numbers of fermions as we did when we created a one-particle state out of the vacuum. The next step is to operate on the single particle state $|\alpha\rangle$ with another

creation operator, a_β, in order to create a two-particle state, i.e.,

$$a_\beta|\alpha\rangle = a_\beta a_\alpha|0\rangle = |\alpha\ \beta\rangle \quad . \tag{2.16}$$

Recall that in the previous section an m-particle state, $|\Gamma\rangle$, was represented by a Slater determinant, as defined in Eq. (2.9), but from here on the state $|\Gamma\rangle$ will be in the operator representation and for m = 2 will equal Eq. (2.16) for the appropriate single particle state labels. Now, when referring to the Slater determinant form, we will replace the l.h.s. of Eq. (2.9) by $|\Gamma\rangle_{s.d.}$.

The ordering of the single particle state labels in Eq. (2.16) is important in that it denotes the order of operation with the creation operators and amounts to specifying phases for our state vectors, however, we are dealing with a system of identical particles and it is impossible to determine the ordering of the occupation of the single particle states because that would present a means of identifying the particles. This means there must be an exchange symmetry of the state labels and since these particles are fermions, the exchange is antisymmetric. Thus we can write

$$|\alpha,\beta\rangle = -|\beta,\alpha\rangle \quad . \tag{2.17}$$

Writing the above equation in terms of creation operators acting upon the vacuum shows us an important relationship, namely,

$$a_\alpha a_\beta + a_\beta a_\alpha = \{a_\alpha, a_\beta\} = 0 \quad . \tag{2.18}$$

Similarly, taking the adjoint of Eq. (2.18) gives us

$$\{b_\alpha, b_\beta\} = 0 \quad . \tag{2.19}$$

To find the relationships between creation and destruction operators, we first use Eqs. (2.18) and (2.19) to show that

$$a_\alpha|\alpha\rangle = 0 \quad \text{and} \quad \langle\alpha|b_\alpha = 0 \quad . \tag{2.20}$$

This is of course just a statement of the Pauli Principle which says that two identical fermions cannot occupy the same state. Next we consider the operation of the destruction operator, b_γ, on a two-particle vector, $|\alpha,\beta\rangle$, namely

$$b_\gamma|\alpha,\beta\rangle \equiv + |\alpha\rangle \quad \text{if} \quad \gamma = \beta \tag{2.21}$$

$$b_\gamma|\alpha,\beta\rangle \equiv - |\beta\rangle \quad \text{if} \quad \gamma = \alpha \quad . \tag{2.22}$$

Even for general m-particle vectors the phase on the r.h.s. can be easily determined by permutating the label of the state that is to become unoccupied to the right most position, then the phase in front of the m-1 particle state is $(-1)^p$, where p is the number of permutations. Finally, if the state is not occupied, then the operation of the destruction operator gives zero, that is,

$$b_\gamma|\alpha,\beta\rangle = 0 \quad \text{if} \quad \gamma \neq \alpha, \neq \beta \quad . \tag{2.23}$$

Considering the products of creation and destruction operators, we can use Eqs. (2.12), (2.13) and (2.14) to show that

$$\begin{aligned} a_\alpha b_\beta|\gamma\rangle &= a_\alpha|0\rangle\delta_{\beta\gamma} \\ &= |\alpha\rangle\delta_{\beta\gamma} \quad . \end{aligned} \tag{2.24}$$

and then we can use Eqs. (2.21) and (2.22) to show that

$$b_\beta a_\alpha |\gamma\rangle = b_\beta |\gamma\alpha\rangle$$
$$= |\gamma\rangle\delta_{\alpha\beta} - |\alpha\rangle\delta_{\alpha\beta} \quad . \tag{2.25}$$

Adding Eqs. (2.24) and (2.25) gives

$$(a_\alpha b_\beta + b_\beta a_\alpha)|\gamma\rangle = |\gamma\rangle\delta_{\alpha\beta} \quad . \tag{2.26}$$

Since $|\gamma\rangle$ is arbitrary, we can write

$$\{a_\alpha, b_\beta\} = \delta_{\alpha\beta} \quad . \tag{2.27}$$

We may summarize all of the anticommutation relations as

$$\begin{aligned} \{a_\alpha, a_\beta\} &= 0 \\ \{b_\alpha, b_\beta\} &= 0 \\ \{a_\alpha, b_\beta\} &= \delta_{\alpha\beta} \quad . \end{aligned} \tag{2.28}$$

A general m-body state vector can be constructed by repeatedly operating on the vacuum with creation operators as is shown by

$$|\alpha, \beta, \ldots, \mu\rangle = a_\mu, \ldots, a_\beta a_\alpha |0\rangle \quad , \tag{2.29}$$

where μ is the label of the m-th occupied state. By applying the anti-commutation relations (2.18) to the r.h.s. of Eq. (2.29), we see that the state vector is antisymmetric under the exchange of any two state labels as it should be.

Taking the adjoint of Eq. (2.29) gives

$$\langle\alpha, \beta, \ldots, \mu| = \langle 0| b_\alpha b_\beta, \ldots, b_\mu \quad . \tag{2.30}$$

If we let

$$\langle\Gamma| \;=\; \langle\alpha,\beta,\ \ldots,\ \mu|$$

be a general m-particle state vector and

$$|\Lambda\rangle \;=\; |\iota,\kappa,\ \ldots,\ \nu\rangle$$

be a general m'-particle state vector, we can write

$$\langle\Gamma|\Lambda\rangle \;=\; \langle 0|b_\alpha b_\beta,\ \ldots,\ b_\mu a_\nu,\ \ldots,\ a_\kappa a_\iota|0\rangle \quad .$$

Using the anticommutation relations (2.28) to move the creation operators to the left will give us m' terms, if m = m', with each single particle state label in $\langle\Gamma|$ contracted with a single particle state label in $|\Lambda\rangle$. If $m \neq m'$, the lesser number of operators will be contracted with an equal number of conjugate operators, leaving (m-m') operators sandwiched between the vacuum. This, of course, gives zero. The normalization of the m-particle states can be stated as

$$\langle\Gamma|\Lambda\rangle \;=\; +\,\delta_{m,m'}(-\,\delta_{m,m'}) \quad , \quad \text{if} \quad (\alpha,\beta,\ \ldots,\ \mu) = (\iota,\kappa,\ \ldots,\ \nu) \tag{2.31}$$

for some even (odd) permutation of labels.

We now discuss the operator representation for a general one-body operator O. We write its operator representation in the following expansion,

$$O' \;=\; \sum_{\alpha\beta} Q_{\alpha\beta} a_\alpha b_\beta \quad , \tag{2.32}$$

where the sum runs over all single particle and we have used a prime to indicate that this operator is in the operator representation. The coefficients $\{Q_{\alpha\beta}\}$ are determined by requiring that the matrix elements

with single particle states in the operator representation equal the corresponding Slater determinant matrix element, ${}_{s.d.}\langle\gamma|0|\delta\rangle_{s.d.}$, that is,

$$ {}_{s.d.}\langle\gamma|0|\delta\rangle_{s.d.} = \sum_{\alpha\beta} Q_{\alpha\beta}\langle 0|b_\gamma a_\alpha b_\beta a_\delta|0\rangle \quad . \tag{2.33} $$

Applying the anticommutation relation (2.28) to permutate the a's to the left gives the contractions $\delta_{\alpha\gamma}\delta_{\beta\delta}$. The sum over all states is thus eliminated leaving $Q_{\gamma\delta}$. Equating this coefficient to the l.h.s. of Eq. (2.33) (in the coordinate representation) shows us that

$$ Q_{\gamma\delta} = \int d^3r_1 \; \phi^+_\gamma(1)\; O(1)\; \phi_\delta(1) \quad , \tag{2.34} $$

where in the r.h.s., $\phi^+_\gamma(1)$ and $\phi_\delta(1)$ are the single particle wavefunctions, O(1) is the one-particle operator acting on the single particle coordinates labeled by (1), including spin and isospin.

A general two-body operator V can be expanded as

$$ V' = \sum_{\substack{\alpha\beta \\ \gamma\delta}} Q_{\alpha\beta\gamma\delta} a_\alpha a_\beta b_\gamma b_\delta \quad , \tag{2.35} $$

where, again, the prime denotes the operator representation. Also, the sum over single particle states is unrestricted. The coefficients $\{Q_{\alpha\beta\gamma\delta}\}$ are determined by requiring that the matrix elements with two particle states in the operator representation equal the Slater determinant matrix elements, ${}_{s.d.}\langle\mu,\eta|V|\iota,\kappa\rangle_{s.d.}$, that is,

$$ {}_{s.d.}\langle\mu,\eta|V|\iota,\kappa\rangle_{s.d.} = \sum_{\substack{\alpha\beta \\ \gamma\delta}} Q_{\alpha\beta\gamma\delta}\langle 0|b_\mu b_\eta a_\alpha a_\beta b_\gamma b_\delta a_\kappa a_\iota|0\rangle \tag{2.36} $$

but again the commutation relation (2.28) allows us to permutate the creation operators to the left leaving the contractions

$$\delta_{\alpha\eta}\delta_{\beta\mu}\delta_{\gamma\iota}\delta_{\delta\kappa} - \delta_{\alpha\eta}\delta_{\beta\mu}\delta_{\gamma\kappa}\delta_{\delta\iota} - \delta_{\alpha\mu}\delta_{\beta\eta}\delta_{\gamma\iota}\delta_{\delta\kappa} + \delta_{\alpha\mu}\delta_{\beta\eta}\delta_{\gamma\kappa}\delta_{\delta\iota} \quad .$$

By taking the sum over α, β, γ, and δ Eq. (3.36) becomes

$$_{s.d.}\langle\mu,\eta|V|\iota,\kappa\rangle_{s.d.} = Q_{\eta\mu\iota\kappa} - Q_{\eta\mu\kappa\iota} - Q_{\mu\eta\iota\kappa} + Q_{\mu\eta\kappa\iota} \quad . \qquad (2.37)$$

Now, the Slater determinant matrix element on the l.h.s. is antisymmetric under permutation of the labels μ and η, or the labels ι and κ, therefore, the r.h.s. is manifestly antisymmetric, but each term on the r.h.s. is not necessarily antisymmetric. We can, in general, write a coefficient as

$$Q_{\pi,\rho,\sigma,\tau} = A_{\pi,\rho,\sigma,\tau} + S_{\pi,\rho,\sigma,\tau} \quad ,$$

where $A_{\pi,\rho,\sigma,\tau}(S_{\pi,\rho,\sigma,\tau})$ is antisymmetric (symmetric) under exchange of the labels π and ρ or the labels σ and τ. Substituting this last equation to Eq. (3.36) and using the appropriate permutation symmetry properties so that (μ,η,ι,κ) is the ordering of labels for each term gives,

$$A_{\pi,\rho,\sigma,\tau} = -\frac{1}{4}\,{}_{s.d.}\langle\mu,\eta|V|\iota,\kappa\rangle_{s.d.} \quad .$$

Note that the symmetric parts of the coefficients have canceled themselves and they do not appear in the last equation. Since there are no more requirements on the coefficients, we are free to set $S_{\pi,\rho,\sigma,\tau} \equiv 0$ for all orbitals. Thus (in the coordinate representation),

$$Q_{\mu\eta\iota\kappa} = -\frac{1}{4}\int\int d^3r_1\, d^3r_2\, \phi_\mu^+(1)\, \phi_\eta^+(2)\, V(1,2)(\phi_\iota(1)\phi_\kappa(2) - \phi_\kappa(1)\phi_\iota(2)) \quad , \tag{2.38}$$

where the two-particle Slater determinants as defined in Eq. (2.9) were written in product form and then the particle labels in two of the terms were exchanged in order to give the more compact form.

One can proceed in this fashion to construct second quantized representations of many body operators. Such representations are especially convenient for performing manipulations that reduce the complexity of traces of many body operators. This is crucial to the application of moment methods in many fermion systems.

C. Nucleon-Nucleon Interaction

The standard method for describing the nucleon-nucleon interaction involves expansions in terms of operators which are invariant under spatial and time displacements and under proper rotations. In addition, they can conserve charge, are symmetric in the two nucleons, conserve parity and are invariant under time reversal. A standard form (8) which fills these requirements is

$$V(\vec{r}) = V_C(r) + V_T(r)S_{12} + V_{SL}(r)\, \vec{L}\cdot\vec{S} \quad , \tag{2.39}$$

where the tensor operator

$$S_{12} \equiv \frac{3(\vec{\sigma}_1\cdot\vec{r})(\vec{\sigma}_2\cdot\vec{r})}{\vec{r}\cdot\vec{r}} - \vec{\sigma}_1\cdot\vec{\sigma}_2 \quad ,$$

r is the distance between the two particles, $\vec{L}$ is the orbital angular momentum, $\vec{\sigma}_1/2$ and $\vec{\sigma}_2/2$ are the spins of each of the particles, and $\vec{S}$

is the total spin. The radial parts, $V_C(r)$, $V_T(r)$ and $V_{LS}(r)$ are usually chosen to be simple functions such as square wells, gaussians, exponentials, or Yukawas, whose parameters are varied to fit the two-nucleon data in the Schroedinger equation.

Reid (8) has used a potential of the form (2.39) with different parameters and slightly different forms for $V_C(r)$, $V_T(r)$, $V_{LS}(r)$ for each partial wave in the nucleon-nucleon system, for total angular momentum not greater than two. The parameters were fit to proton-proton scattering phase shifts for the isospin one channel and to proton-neutron scattering phase shifts as well as deuteron properties for the isospin zero channel. He developed two sets of potentials, one which becomes infinitely repulsive inside a critical distance, and one which remains finite but is large and repulsive at distances approaching zero. In this work we will use the latter set, called the soft core potential, for the two-nucleon interaction.

D. Effective Hamiltonian

We will derive the effective Hamiltonian by writing the many body Schroedinger equation,

$$H|B\rangle = E_B|B\rangle \quad , \tag{2.4}$$

for d of the states and eigenenergies, in terms of a finite shell model basis, $\{|\Gamma\rangle\}$, as described in Section A. First we divide the shell model basis up into two subspaces; a finite part with $\Gamma = 1, \ldots, d$, and an infinite part with $\Gamma = d+1, \ldots, \infty$. For projecting into the finite basis we define the projection operator

$$P = \sum_{\Gamma=1}^{d} |\Gamma\rangle\langle\Gamma| \tag{2.40}$$

and into the complementary space the operator

$$Q = \sum_{\Gamma=d+1}^{\infty} |\Gamma\rangle\langle\Gamma| \quad . \tag{2.41}$$

The completeness relation,

$$\sum_{\Gamma=1}^{\infty} |\Gamma\rangle\langle\Gamma| = 1 \quad ,$$

can then be written as

$$P + Q = 1 \quad . \tag{2.42}$$

If the operator O in Eq. (2.1) is taken to be the total kinetic energy operator, then by adding and subtracting

$$U = \sum_{i=1}^{m} u(i) \quad ,$$

where u(i) is the one body interaction in Eq. (2.6), we can write

$$H = H_O + H_I \tag{2.43}$$

where

$$H_O = O + U$$

and

$$H_I = O - U \quad .$$

Next we operate on Eq. (2.4) with Eqs. (2.40), (2.41) and (2.42) in order to derive the Schroedinger equation for the finite model space,

$$H(E_C)\ P|C\rangle = E_C\ P|C\rangle \quad . \tag{2.44}$$

This equation can be solved for d of the eigenvalues in Eq. (2.4) but not necessarily the lowest d eigenvalue because there is now no way to determine the ordering of the states. The wavefunctions $P|C\rangle$ are projections of d of the states $|C\rangle$ onto the finite shell model space. The effective Hamiltonian in (2.44) is

$$H(E_C) = PH_0P + PV(E_C)P \tag{2.45}$$

where

$$V(E_C) = H_I + \frac{H_I Q H_I}{E_C - QHQ} \quad . \tag{2.46}$$

The identity

$$\frac{1}{A+B} = \frac{1}{A} - \frac{1}{A}\,B\,\frac{1}{A+B} \tag{2.47}$$

can be used to expand H_I out of the denominator giving

$$V(E_C) = H_I + H_I \frac{Q}{E_C - H_0} V(E_C) \quad . \tag{2.48}$$

This last equation is known as the Brillouin-Wigner expansion but because it is dependent on the unknown energy, E_C, this form of the theory is not usually practical to work with, unless some self-consistent approach is taken.

For the case where all single particle energies, ε_α, in the finite shell model basis are degenerate, the energy dependence can be removed from the interaction, as shown by Brandow and others (9 ,10,11) giving a Rayleigh-Schroedinger expansion called the linked-folded (LF) series,

$$V = \left[H_I + H_I \frac{QV}{E - H_0} \right]_{LF} , \qquad (2.49)$$

where $E = m\varepsilon_\alpha$ for this degenerate case..

Many of the nucleon-nucleon interactions that are used have a large, repulsive core. This makes calculations of Eq. (2.49) to any order impractical because the two-body matrix elements of V(i,j) are then too large to work with directives. This problem can be handled by first solving the iterated equation, known as the Bethe-Goldstone equation (12),

$$G(\omega) = V + \frac{V\, Q_{2p}\, G(\omega)}{(\omega - H_0)} , \qquad (2.50)$$

where Q_{2p}, the Pauli blocking operator, projects onto a two-particle subspace of Q states where either one or both of the interacting particles occupy an orbit outside of the finite shell model space. The parameter ω is known as the starting energy and takes into account the fact that the nucleons are interacting not in free space, but inside the nucleus. It is chosen as the average interaction energy (negative) of two particles in the model space. The effective interaction (2.49) can be resumed as

$$V = \left[G + \frac{G\bar{Q}G}{E - H_0} \right]_{LF} , \qquad (2.51)$$

where $\bar{Q}$ is a many-body projection operator like Q except that all projections involving two-particle states which are already iterated into G are excluded. All terms in Eq. (2.49) with U in the numerator, including in the first term in Eq. (2.45), can be treated separately in a perturbation series or largely eliminated through a self-consistent approach (6). One can then go on to solve Eq. (2.51) to the highest order possible in G (13).

Since our shell model states can possibly include particles occupying states with different single-particle energies, the theory can become nondegenerate in nature. This can be handled within the degenerate theory that we have already discussed by perturbatively treating the degeneracy breaking terms (14). We could avoid this difficulty, however, by using an average value for E, thus assuming a degeneracy among the single-particle states in an average sense. This is simply a matter of choosing a point about which our expansions are made and does not represent an approximation as long as convergence is achieved.

Because of the nature of Eq. (2.50), we would hope that with a large enough model space, the use of G alone for the effective interaction would be sufficient. This, applied to the fact that the calculation of any higher order terms in Eq. (2.51) becomes extremely difficult, leads us to write

$$H = P(0 + V)P \rightarrow P(0 + G)P \tag{2.52}$$

as the effective Hamiltonian with which we will work.

Finally, we partially eliminate the energy due to spurious center of mass motion by subtracting the center of mass kinetic energy out of the effective Hamiltonian, that is

$$H \rightarrow H - P\, T_{CM}\, P \quad . \tag{2.53}$$

Since the total kinetic energy can be written as

$$0 = T_{CM} + T_{Rel} \quad , \tag{2.54}$$

where

$$T_{rel} = \frac{1}{m} \sum_{i,j=1}^{m} \frac{p_{ij}^2}{2\mu} \quad , \tag{2.55}$$

as derived in Appendix B, we have

$$H = P(T_{Rel} + G)P \tag{2.56}$$

as our effective Hamiltonian.

In the above treatment $|0\rangle$ was defined as the vacuum or reference state. The formalism is thus equally applicable to situations where we start the perturbation series by assuming a passive core of nucleons in lowest order as well as to cases where no-core is assumed. A particular feature of the applications performed here is the emphasis on no-core studies.

E. Phenomenological Effective Interactions

Because the effective interaction discussed in the previous section is extremely difficult to calculate, even to lowest order in G, phenomenological effective interactions have been constructed for the sake of simplifying shell model calculations. A number of them (15) can be written as expansions in terms of their components in spin and isospin space, that is,

$$V(r) = V_{00}(r)P^{00} + V_{10}(r)P^{10} + V_{01}(r)P^{01} + V_{11}(r)P^{11} \quad , \quad (2.57)$$

where r is the separation between the two interacting particles, the sub- and superscripts are the spin and isospin subspace identifiers, respectively, and P^{ST} is the spin-isospin projection operator.

An approximation to the G matrix, which is of the form of Eq. (2.57), has been developed by Kallio-Kolltveit (16). They start with

$$V(r) = V_T(r)P^{10} + V_S(r)P^{01} \quad ,$$

which involves the relative S-wave only, and has radial dependence,

$$V_k(r) = \begin{cases} -A_k \, e^{-\alpha_k(r-c_k)} & r \geq c \\ \infty & r < c \end{cases} \quad . \quad (2.58)$$

They fit the parameters,

	C_k(fm)	A_k(MeV)	α_k(fm^{-1})
triplet	0.4	475.0	2.5214
singlet	0.4	330.8	2.4021

to the scattering length and binding energy of the deuteron.

Finally, they apply the method of separation of Scott and Moszkowski (17) which, in lowest order, approximates

$$G(r) \approx V(r) \quad . \tag{2.59}$$

Now, however,

$$V_k = \begin{cases} -A_k \, e^{-\alpha_k (r-C)} & r \geq d_k > C \\ 0 & r < d_k \end{cases} ,$$

where the separation distance, d_k, as determined by the method of separation, is .925 fm for the triplet term and 1.025 fm for the singlet term. This is, in effect, a method for removing the hard core from the nucleon-nucleon interaction, and as discussed in the previous section, the effective interaction was re-defined in terms of an exact G matrix (2.50) in order to treat this very problem.

III. MOMENT METHODS

We begin this chapter with a discussion of the definition of traces and moments of operating including subspace traces and moments. In the second section we will discuss methods for evaluating many-body traces of operators which involves summations of contracted single-particle state labels of one and two-body matrix elements. In this section we also include the evaluation of configuration traces. In Section C we will discuss the evaluation of the expectation value of a general operator using trace techniques, in terms of orthogonal polynomial expansions.

A. Definitions of Traces and Moments

We are interested in calculating the trace of an operator K which is the product of one and two-body operators;

$$K = O_1(k_1), O_2(k_2), \ldots, O_i(k_i), \ldots O_\ell(k_\ell) \tag{3.1}$$

where $O_i(k_i)$ is a k_i-body (one or two-body) operator in the product K. For the trace of K over a finite space S we use the following notation

$$\langle\langle K \rangle\rangle_S = \sum_{B=1}^{d} \langle B|K|B\rangle \quad . \tag{3.2a}$$

The moment of K is given by

$$\langle K \rangle_S = \frac{\langle\langle K \rangle\rangle_S}{d} \quad , \tag{3.2b}$$

where

$$S = \{|B\rangle, B=1, \ldots, d\} \tag{3.2c}$$

is an orthonormal basis of dimensionality d.

We can expand S in terms of another orthonormal basis $S' = \{|\Gamma\rangle, \Gamma=1, \ldots, d\}$ by a similarity transformation;

$$|B\rangle = \sum_{\Gamma=1}^{d} a_{B\Gamma}|\Gamma\rangle \quad ,$$

where

$$\sum_{B=1}^{d} a^{*}_{\Lambda B}\, a_{B\Gamma} = \delta_{\Lambda\Gamma} \quad .$$

Placing this transformation into Eq. (3.2) gives the well-known invariance property of a trace. That is

$$\begin{aligned} \langle\langle K\rangle\rangle_S &= \sum_{\Gamma=1}^{d} \sum_{\Lambda=1}^{d} \sum_{B=1}^{d} a^{*}_{\Lambda B}\, a_{B\Gamma} \langle\Lambda|K|\Gamma\rangle \quad , \\ &= \sum_{\Gamma=1}^{d} \langle\Gamma|K|\Gamma\rangle \\ &= \langle\langle K\rangle\rangle_{S'} \quad . \end{aligned} \tag{3.3}$$

It is this invariance property that allows us to choose a convenient representation in which to work.

Writing the trace of K over S' as trace of the product of operators,

$$\langle\langle O_1 O_2, \ldots O_\ell\rangle\rangle_{S'} = \sum_{\Gamma=1}^{d} \langle\Gamma|O_1 O_2, \ldots, O_\ell|\Gamma\rangle \quad ,$$

and then inserting the completeness relation,

$$\sum_{\Lambda=1}^{d} |\Lambda\rangle\langle\Lambda| = 1 \quad ,$$

between the first two operators gives us

$$\langle\langle O_1 O_2, \ldots, O_\ell \rangle\rangle_{S'} = \sum_{\substack{\Gamma=1 \\ \Lambda=1}}^{d} \langle\Gamma|O_1|\Lambda\rangle\langle\Lambda|O_2, \ldots, O_\ell|\Gamma\rangle \quad .$$

By permuting the matrix element, $\langle\Gamma|O_1|\Lambda\rangle$, to the right side of the equation and again using the completeness relation summed over the states labeled Γ, we see that

$$\begin{aligned} \langle\langle O_1 O_2, \ldots, O_\ell \rangle\rangle_{S'} &= \sum_{\Lambda=1}^{d} \langle\Lambda|O_2, \ldots, O_\ell O_1|\Lambda\rangle \\ &= \langle\langle O_2, \ldots, O_\ell O_1 \rangle\rangle_{S'} \quad . \end{aligned} \tag{3.4}$$

The procedure can be repeated to show that the trace over S' of the product of operators is invariant under any cyclic permutation of the operators in the product.

It is possible that one may be interested in the trace of K over a subspace of S where all of the states have the same good quantum number for some symmetry property such as the z-component of the total angular momentum J_z. Consider an operator R (which could be the operator J_z) for which the states of S are eigenvectors then

$$R|B_i\rangle = r_i|B_i\rangle$$

where r_i is one of a set of k eigenvalues and i = 1, ..., k. The subspace S_i is then defined as

$$S_i = \{|B_i\rangle\}$$

so that

$$S = S_i \cup S_2 \cup \ldots \cup S_k$$

but

$$\phi = S_i \cap S_j \quad , \quad \text{all } i,j = 1, 2, \ldots, k \quad ,$$

where ϕ is the null set.

We define the subspace trace of K over S_i as

$$\langle\langle K\rangle\rangle_{S_i} = \sum_{B_i \epsilon S_i} \langle B_i|K|B_i\rangle \quad , \tag{3.5}$$

and the subspace moment of K as

$$\langle K\rangle_{S_i} = \langle\langle K\rangle\rangle_{S_i}/d_i \quad , \tag{3.6}$$

where d_i is the number of states in S_i. With the definition in Eq. (3.5), we see that if we partition the sum in Eq. (3.2) over all the k subspaces of S, we will get

$$\langle\langle K\rangle\rangle_S = \sum_{i=1}^{k} \sum_{B_i \epsilon S_i} \langle B_i|K|B_i\rangle$$

$$= \sum_{i=1}^{k} \langle\langle K\rangle\rangle_{S_i} \quad . \tag{3.7}$$

By substituting K = 1 in Eq. (3.6), we find that

$$d = \langle\langle 1\rangle\rangle_S$$

$$= \sum_{i=1}^{k} \langle\langle 1 \rangle\rangle_{S_i} = \sum_{i=1}^{k} d_i \quad . \tag{3.8}$$

Let the states of S' (again, for example, the states of S' could also exhibit good J_z) also be eigenstates of the opertor R_i, that is

$$R|\Gamma_j\rangle = t_j|\Gamma_j\rangle \quad ,$$

where t_j is one of a set of ℓ eigenvalues and $j = 1, \ldots, \ell$. It can be shown that when there is a unitary transformation such that

$$|B\rangle = \sum_{\Gamma=1}^{d} a_{B\Gamma}|\Gamma\rangle \quad ,$$

then for each subspace S_i, there will correspond a subspace S_j' such that their quantum numbers equal, i.e., $t_i = t_j$. Also, the states in these corresponding subspaces will transform unitarily, that is

$$|B_i\rangle = \sum_{\Gamma \epsilon S_i'} a^i_{B\Gamma}|\Gamma_i\rangle \tag{3.9}$$

and

$$\sum_{B_i \epsilon S_i} a^*_{\Lambda_i B_i} a_{B_i \Gamma_i} = \delta_{\Lambda_i \Gamma_i} \quad , \tag{3.10}$$

where we have now relabeled each subspace in S' with the label i of its corresponding space in S. (For example, for each subspace in S with the good quantum number J_z, there exists a subspace in S' with the same good quantum number, and we have given these two corresponding subspaces the same label.)

If we expand the vector $|B_i\rangle$ and its adjoint in Eq. (3.5) in terms of the basis S_i' in Eq. (3.9), and apply the condition in Eq. (3.10), we see that

$$\begin{aligned} \langle\langle K \rangle\rangle_{S_i} &= \sum_{\Gamma_i \epsilon S_i} \langle \Gamma_i | K | \Gamma_i \rangle \\ &= \langle\langle K \rangle\rangle_{S_i'} \quad , \quad i = 1, \ldots, \ell \quad . \end{aligned} \tag{3.11}$$

In general, the above equation is not true. One can partition the space S into subspaces where no symmetry of the eigenvectors is employed in the partitioning. Such a trace over a subspace (i.e., a partial trace) is <u>not</u> invariant under a unitary transformation. It is important to keep this in mind for applications involving configuration expansions.

B. Trace Reduction Formulae

We need to calculate traces of products of operators over a finite shell model basis

$$S(m) = \{ |\Gamma\rangle, \Gamma=1, \ldots, d_m \} \quad . \tag{3.12}$$

This basis is composed of m-particle Slater determinants which are defined in Eq. (2.9). Each Slater determinant is an antisymmeterized product of m single-particle states and the m single-particle state labels are chosen from a set of N single particle state labels. There are $\binom{N}{m}$ ways to fill N orbitals with m identical particles and this is the dimensionality d_m of S(m).

The <u>scalar trace</u> of an operator K, which is defined in Eq. (2.1), is defined as

$$\langle\langle K \rangle\rangle_{S(m)} = \sum_{\Gamma=1}^{d_m} \langle \Gamma | K | \Gamma \rangle \quad , \tag{3.13}$$

where the sum is taken over <u>all</u> states in S(m).

For the scalar trace of a one-body operator, O(1), which is defined in Eqs. (2.32) and (2.34), we write

$$\langle\langle O(1) \rangle\rangle_{S(m)} = \sum_{\Gamma=1}^{d_m} \sum_{\alpha\beta} O_{\alpha\beta} \langle \Gamma | a_\alpha b_\beta | \Gamma \rangle \quad . \tag{3.14}$$

We can apply Eqs. (2.29) and (2.30) in order to write the diagonal matrix element as

$$\langle \Gamma | a_\alpha b_\beta | \Gamma \rangle = \langle 0 | b_h \ldots b_i \ldots b_m (a_\alpha b_\beta) a_m \ldots a_i \ldots a_h | 0 \rangle \quad ,$$

where we have used the lower case Roman subscripts to denote the occupied orbitals in the state Γ. Wick's theorem, which is discussed in Appendix A, can be applied to reduce the above equation to the contractions

$$\langle \Gamma | a_\alpha b_\beta | \Gamma \rangle = \sum_{i \varepsilon S(\Gamma)} \delta_{i\alpha} \, \delta_{\alpha\beta}$$

where the sum is taken over each of the occupied single-particle orbitals i that belong to the m-particle state Γ. Replacing the diagonal matrix element in Eq. (3.14) with this sum of contractions and then summing over the label β, we see that

$$\langle\langle O(1) \rangle\rangle_{S(m)} = \sum_{\Gamma=1}^{d_m} \sum_{\alpha} O_{\alpha\alpha} \sum_{i \varepsilon S(\Gamma)}^{m} \delta_{i\alpha} \quad .$$

From each m-particle state Γ, the sum over i will be zero unless the state α is an occupied state in Γ, so that we can write the trace as

$$\langle\langle O(1)\rangle\rangle_{S(m)} = \sum_{\Gamma=1}^{d_m} \sum_{\alpha} O_{\alpha\alpha}\, \Delta(\alpha;\Gamma) \quad , \tag{3.15}$$

where $\Delta(\alpha;\Gamma)$ is defined as 1(0) depending upon whether α is (is not) an occupied single-particle state in Γ. All N single-particle states are treated equally when occupying m of them at a time in all possible ways in order to construct the m-particle basis states, and because of this each single particle state will be occupied a multiple R of times in the $\binom{N}{m}$ m-particle states. Because of this multiple occurrence in the double sum, the sum over Γ with the function $\Delta(\alpha;\Gamma)$ in Eq. (3.15) can be replaced (Appendix C) by the factor $R = \binom{N}{m}\binom{m}{1}/\binom{N}{1} = \binom{N-1}{m-1}$, where $\binom{N}{m}$ is the number of m-particle states in the sum over Γ, $\binom{m}{1}$ is the number of one-particle states whose labels appear in each m-particle state, and $\binom{N}{1}$ is the number of one-particle states that are created by occupying a set of N states, one at a time. Thus the trace of O(1) can be written as

$$\langle\langle O(1)\rangle\rangle_{S(m)} = \binom{N-1}{m-1} \sum_{\alpha} O_{\alpha\alpha} \quad . \tag{3.16}$$

For the scalar trace of a two-body operator O(2), which is defined in Eqs. (2.35) and (2.37), we write

$$\langle\langle O(2)\rangle\rangle_{S(m)} = \sum_{\Gamma=1}^{d_m} \sum_{\alpha\beta\gamma\delta} O_{\alpha\beta\gamma\delta} \langle\Gamma| a_\alpha a_\beta b_\gamma b_\delta |\Gamma\rangle \quad . \tag{3.17a}$$

We can apply Eqs. (2.29) and (2.30) in order to write the diagonal matrix element in (3.17a)

$$\langle\Gamma|a_\alpha a_\beta b_\gamma b_\delta|\Gamma\rangle = \langle 0|b_h \ldots b_i \ldots b_m(a_\alpha a_\beta b_\gamma b_\delta)a_m \ldots a_j \ldots a_i \ldots a_h|0\rangle,$$

where we have used lower case Roman subscripts to denote the occupied orbitals in the state Γ. Wick's theorem, which is discussed in Appendix A, can be applied to the right hand side of the above equation in order to reduce the equation to the following:

$$\langle\Gamma|a_\alpha a_\beta b_\gamma b_\delta|\Gamma\rangle = \sum_{(i,j)\varepsilon S(\Gamma)} (\delta_{j\alpha}\delta_{i\beta}\delta_{\alpha\delta}\delta_{\beta\gamma} + \delta_{i\alpha}\delta_{j\beta}\delta_{\alpha\delta}\delta_{\beta\gamma} - \delta_{i\alpha}\delta_{j\beta}\delta_{\alpha\gamma}\delta_{\beta\delta} - \delta_{j\alpha}\delta_{i\beta}\delta_{\alpha\gamma}\delta_{\beta\delta} \quad ,$$

where the sum is taken over all pairs of single-particle orbitals in the state Γ.

After replacing the diagonal matrix element in Eq. (3.17) with this sum of contractions, summing over γ and δ, and then using the antisymmetric property $O_{\alpha\beta\beta\alpha} = -O_{\alpha\beta\alpha\beta}$, we can write the trace of O(2) as

$$\langle\langle O(2)\rangle\rangle_{S(m)} = \sum_{\Gamma=1}^{d_m} \sum_{\alpha\beta} 2\, O_{\alpha\beta\beta\alpha} \sum_{(i,j)\varepsilon S(\Gamma)} (\delta_{j\alpha}\delta_{i\beta} + \delta_{i\alpha}\delta_{j\beta}) \quad . \quad (3.17b)$$

Because of contractions, the sum over all pairs of occupied orbitals in Γ, will be zero unless α and β are occupied in Γ, and so we can write Eq. (3.17b) as

$$\langle\langle O(2)\rangle\rangle_{S(m)} = \sum_{\Gamma=1}^{d_m} \sum_{\alpha\beta} 2\, O_{\alpha\beta\beta\alpha}\, \Delta(\alpha,\beta;\Gamma) \quad , \quad (3.18)$$

where the function $\Delta(\alpha,\beta;\Gamma)$ is defined as 1 if α and β are both occupied in the state Γ, and is equal to 0 otherwise.

Finally, the sum over Γ with the function $\Delta(\alpha,\beta;\Gamma)$ can be replaced (Appendix C) by the multiple occurrence factor $R = \binom{N}{m}\binom{m}{2}\binom{N}{2} = \binom{N-2}{m-2}$, where $\binom{N}{m}$ is the number of m-particle states in the sum over Γ, $\binom{m}{2}$ is the number of two-particle states whose labels appear in each m-particle state, and $\binom{N}{2}$ is the number of two-particle states that are constructed by occupying a set of N states two at a time. Thus the trace of O(2) can be written as

$$\langle\langle O(2)\rangle\rangle_{S(m)} = \binom{N-2}{m-2} 2 \sum_{\alpha\beta} O_{\alpha\beta\beta\alpha} \quad . \tag{3.19}$$

For the scalar trace of the square of a one-body operator $O^2(1)$, we can use the anticommutation relations in Eq. (2.28) to write

$$\begin{aligned} O^2(1) &= \sum_{\alpha\beta\gamma\delta} O_{\alpha\beta}O_{\gamma\delta}a_\alpha b_\beta a_\gamma b_\delta \\ &= \sum_{\alpha\beta\gamma\delta} O_{\alpha\beta}O_{\gamma\delta}a_\alpha(\delta_{\beta\gamma} - a_\gamma b_\beta)b_\delta \\ &= \sum_{\alpha\delta}\Big(\sum_{\beta} O_{\alpha\beta}O_{\beta\delta}\Big)a_\alpha b_\delta - \sum_{\alpha\beta\gamma\delta} O_{\alpha\beta}O_{\gamma\delta}a_\alpha a_\gamma b_\beta b_\delta \\ &= \bar{O}(1) + \bar{O}(2) \quad . \end{aligned} \tag{3.20}$$

Thus, the scalar trace of $O^2(1)$ can be written as

$$\langle\langle O^2(1)\rangle\rangle_{S(m)} = \langle\langle \bar{O}(1)\rangle\rangle_{S(m)} + \langle\langle \bar{O}(2)\rangle\rangle_{S(m)} \quad . \tag{3.21}$$

The first term in Eq. (3.21) is determined in the same way as the scalar trace for the one-body operator O(1), and we have already calculated this with the result given in Eq. (3.16). Therefore, for the first term in Eq. (3.21) we can write

$$\langle\langle \bar{O}(1) \rangle\rangle_{S(m)} = \binom{N-1}{m-1} \sum_{\alpha} \bar{O}_{\alpha\alpha}$$

$$= \binom{N-1}{m-1} \sum_{\alpha\beta} O_{\alpha\beta} O_{\beta\alpha} \quad . \tag{3.22}$$

The second term in Eq. (3.21) is determined in the same manner as the scalar trace for the two-body operator O(2), except that now the antisymmeterization property of the coefficients does not hold, that is, $\bar{O}_{\alpha\beta\beta\alpha} \neq -\bar{O}_{\alpha\beta\alpha\beta}$. If we replace 2 $O_{\alpha\beta\beta\alpha}$ by $\bar{O}_{\alpha\beta\beta\alpha} - \bar{O}_{\alpha\beta\alpha\beta}$ in Eq. (3.19), then we can write

$$\langle\langle \bar{O}(2) \rangle\rangle = \binom{N-2}{m-2} \sum_{\alpha\beta} (\bar{O}_{\alpha\beta\beta\alpha} - \bar{O}_{\alpha\beta\alpha\beta})$$

$$= \binom{N-2}{m-2} \sum_{\alpha\beta} O_{\alpha\alpha} O_{\beta\beta} - \binom{N-2}{m-2} \sum_{\alpha\beta} O_{\alpha\beta} O_{\beta\alpha} \quad . \tag{3.23}$$

Finally, by placing Eqs. (3.22) and (3.23) into Eq. (3.21) and using the identity $\binom{N-1}{m-1} - \binom{N-2}{m-2} = \binom{N-2}{m-1}$, we can write the scalar trace of $O^2(1)$ as

$$\langle\langle O^2(1) \rangle\rangle_{S(m)} = \binom{N-2}{m-1} \sum_{\alpha\beta} O_{\alpha\beta} O_{\beta\alpha} + \binom{N-2}{m-2} \sum_{\alpha\beta} O_{\alpha\alpha} O_{\beta\beta} \quad . \tag{3.24}$$

For a k-body operator O(k) which is represented with k creation operations to the left of k destruction operators, we can generalize the above results (Appendix C) to obtain for the scalar trace

$$\langle\langle O(k) \rangle\rangle_{S(m)} = \binom{N-k}{m-k} \langle\langle O(k) \rangle\rangle_{S(k)} \quad , \tag{3.25}$$

where S(k) is the finite shell model basis of k-particle states, and it is constructed by occupying the set of N single-particle orbitals k orbitals at a time, in all possible ways.

For a general operator K, where

$$K = O(k_1)O(k_2), \ldots, O(k_\ell) \quad , \tag{3.26}$$

we can always use the anticommutation relations, which are given in Eq. (2.28), to commute all of the creation operators to the left of the destruction operators, creating contractions of single-particle labels as we do so. As a result, we can write K as

$$K = \sum_{k=0}^{k'} \bar{O}(k) \quad , \quad k' = k_1 + k_2 + \ldots + k_\ell \quad . \tag{3.27}$$

(An example of this redefinition of the product operator K is seen earlier in this section, in the derivation of the scalar trace of the operator $O^2(1)$, where we rewrote $O^2(1)$ as $\bar{O}(1) + \bar{O}(2)$.) We can then apply Eq. (3.25) to each term in Eq. (3.27) to write the scalar trace of the product operator K as

$$\langle\langle K \rangle\rangle_{S(m)} = \sum_{k=0}^{k'} \binom{N-k}{m-k} \langle\langle \bar{O}(k) \rangle\rangle_{S(k)} \quad . \tag{3.28}$$

In practice, however, even the k-body traces $\langle\langle O(k) \rangle\rangle_{S(k)}$ in Eq. (3.28) will be difficult if k gets larger than two. For dealing with more difficult traces of products of operators, one can use the following Ginocchio trace reduction formula (3,18,19) which deals directly with sums over contracted single particle labels:

$$\langle\langle K \rangle\rangle_{S(m)} = \sum_{t} \binom{N-k}{m-t} D_t^k(K) \quad , \tag{3.29}$$

where the basic diagrams $D_t^k(K)$ are determined by taking all possible

full contractions between the k creation and k destruction operators, and $0 \leq t \leq$ smaller (k,m). In each basic diagram, t contractions will be left contractions, where the creation operators lie to the left of the contracted destruction operators. (In addition, each fully contracted term will have a phase factor of +1 or -1 depending upon whether an even or odd (respectively) number of permutations of operators is required to bring each of the contracted pairs together.)

For the simplest case, where $K = O(1)$, there is only one possible contraction, $\overbrace{a_\alpha b_\beta}$, and it is a left contraction. Thus, we write that

$$D_1^1(O(1)) = \sum_\alpha O_{\alpha\alpha} \quad ,$$

and the trace becomes

$$\langle\langle O(1)\rangle\rangle_{S^1(m)} = \binom{N-1}{m-1} \sum_\alpha O_{\alpha\alpha} \quad ,$$

which agrees with Eq. (3.16).

For the case where $K = O(2)$, there are two contractions $\overbrace{a_\alpha a_\beta b_\gamma b_\delta}$ and $\overbrace{a_\alpha a_\beta b_\gamma b_\delta}$, and they are both left contractions. Thus, we can write

$$D_2^2(O(2)) = \sum_{\alpha\beta} (O_{\alpha\beta\beta\alpha} - O_{\alpha\beta\alpha\beta}) = 2 \sum_{\alpha\beta} O_{\alpha\beta\beta\alpha} \quad ,$$

where use was made of the permutation symmetry of the coefficients, that is

$$O_{\alpha\beta\alpha\beta} = -O_{\alpha\beta\beta\alpha} \quad .$$

The trace is then

$$\langle\langle O(2)\rangle\rangle_{S(m)} = \binom{N-2}{m-2} 2 \sum_{\alpha\beta} O_{\alpha\beta\beta\alpha} \quad ,$$

which agrees with Eq. (3.19).

For the case where $K = O^2(1)$, there are two contract ions. The first contraction, $\overbrace{a_\alpha b_\beta} \overbrace{a_\gamma b_\delta}$, contains two left contractions and the basic diagram is

$$D_2^2(O^2(1)) = \sum_{\alpha\beta} O_{\alpha\alpha} O_{\beta\beta} \quad .$$

The second contraction, $\overbrace{a_\alpha \overbrace{b_\beta a_\gamma} b_\delta}$, contains only one left contraction and the basic diagram is

$$D_1^2(O^2(1)) = \sum_{\alpha\beta} O_{\alpha\beta} O_{\beta\alpha} \quad .$$

Placing the two basic diagrams into Eq. (3.24), we can then write the scalar trace of $O^2(1)$ as

$$\langle\langle O^2(1)\rangle\rangle_{S(m)} = \binom{N-2}{m-1} \sum_{\alpha\beta} O_{\alpha\beta} O_{\beta\alpha} + \binom{N-2}{m-2} \sum_{\alpha\beta} O_{\alpha\alpha} O_{\beta\beta} \quad .$$

This agrees with the result obtained in Eq. (3.24) where we only used Wick's theorem for the answer.

For the case where

$$K = O^2(2)$$

$$= \sum_{\substack{\alpha,\beta,\gamma,\delta \\ \mu,\nu,\zeta,\eta}} O_{\alpha\beta\gamma\delta} O_{\mu\nu\zeta\eta} a_\alpha a_\beta b_\gamma b_\delta a_\mu a_\nu b_\zeta b_\eta \quad ,$$

there are 4! contractions between the four creation and destruction

operators. For each of the basic diagrams for $O^2(2)$ the symmetry properties of the two-body coefficients can be used to show that all terms are alike.

There are four like terms with four left contractions so this basic diagram is

$$D_4^4(O^2(2)) = 4 \sum_{\alpha,\beta,\gamma,\delta} O_{\alpha\beta\beta\alpha} O_{\gamma\delta\delta\gamma}$$

$$= 4\Big(\sum_{\alpha\beta} O_{\alpha\beta\beta\alpha} \Big)^2 \quad . \tag{3.30}$$

There are sixteen like terms with three left contractions so this basic diagram is

$$D_3^4(O^2(2)) = 16 \sum_{\alpha,\beta,\gamma,\delta} O_{\alpha\beta\beta\gamma} O_{\gamma\delta\delta\alpha} \quad . \tag{3.31}$$

Finally, there are four like terms with two left contractions, and this basic diagram is

$$D_2^4(O^2(2)) = 4 \sum_{\alpha,\beta,\gamma,\delta} O_{\alpha\beta\gamma\delta} O_{\delta\gamma\beta\alpha}$$

$$= 4 \sum_{\alpha,\beta,\gamma,\delta} (O_{\alpha\beta\gamma\delta})^2 \quad , \tag{3.32}$$

where the last equality becomes true if we are dealing with symmetric matrix elements. Thr trace of $O^2(2)$ is, therefore,

$$\langle\langle O^2(2)\rangle\rangle_{S(m)} = \binom{N-4}{m-4} 4\Big(\sum_{\alpha\beta} O_{\alpha\beta\beta\alpha} \Big)^2 + \binom{N-4}{m-3} 16 \sum_{\alpha,\beta,\gamma,\delta} O_{\alpha\beta\beta\gamma} O_{\gamma\delta\delta\alpha}$$

$$+ \binom{N-4}{m-2} 4 \sum_{\alpha,\beta,\gamma,\delta} (O_{\alpha\beta\gamma\delta})^2 \quad .$$

In the finite shell model basis, S(m), a <u>configuration</u> subspace is created by first partitioning the N single particle orbitals in to ℓ parts, with N_i orbitals in the i-th subspace, so that $\sum_{i=1}^{\ell} N_i = N$. A particular configuration subspace is designated by $S(\vec{m})$, where $\vec{m} = (m_1, m_2, \ldots, m_\ell)$, $m_1 \leq N_1$, etc., and $\sum_{i=1}^{\ell} m_i = m$. In this particular configuration, m_i identical particles are restricted to occupy the N_i orbitals of the i-th partition in all possible ways, giving $\binom{N_i}{m_i}$ combinations. By taking all such possible combinations in all subspaces into account, we see that the dimensionality of $S(\vec{m})$ is

$$d_{\vec{m}} = \prod_{i=1}^{\ell} \binom{N_i}{m_i} \quad . \tag{3.33}$$

For a given partitioning $(N_1, N_2, \ldots, N_\ell)$ of the single-particle orbitals, the union of all configuration subspaces $S(\vec{m})$, which are made from all possible $\vec{m}$ such that $m_1 + \ldots + m_\ell = m$, is the full finite shell model space, S(m). If we look at the dimensionality $d_m = \binom{N}{m}$ of S(m), and then use Vandermonde's theorem (20) to show that

$$\binom{N}{m} = \sum_{\substack{m_1,\ldots,m_\ell \\ m_1+\ldots+m_\ell=m}} \prod_{i=1}^{\ell} \binom{N_i}{m_i} = \sum_{\vec{m}} d_{\vec{m}} \quad ,$$

we see that, indeed,

$$d_m = \sum_{\vec{m}} d_{\vec{m}} \quad .$$

We will define a configuration trace as

$$\langle\langle K\rangle\rangle_{S(\vec{m})} = \sum_{\Gamma \epsilon S(\vec{m})} \langle\Gamma|K|\Gamma\rangle \quad , \tag{3.34}$$

and a configuration moment as

$$\langle K\rangle_{S(\vec{m})} = \langle\langle K\rangle\rangle_{S(\vec{m})}/d_{\vec{m}} \quad . \tag{3.35}$$

Because the full space S(m) is the union of all configuration subspaces $S(\vec{m})$, we can write the scalar trace of K as the sum of all configuration traces, that is,

$$\langle\langle K\rangle\rangle_{S(m)} = \sum_{\vec{m}} \langle\langle K\rangle\rangle_{S(\vec{m})} \quad . \tag{3.36}$$

For the configuration trace of a one-body operator O(1), where the N single-particle orbitals are partitioned into two parts with N_1 orbitals in the first partition and N_2 orbitals m_2 in the second partition and m_1 orbitals are occupied in the first partition and m_2 are occupied in the second partition, we write

$$\langle\langle O(1)\rangle\rangle_{S(m_1,m_2)} = \sum_{\Gamma \epsilon S(m_1,m_2)} \sum_{\alpha\beta} O_{\alpha\beta} \langle\Gamma|a_\alpha b_\beta|\Gamma\rangle \quad .$$

We found in the example for the scalar trace of O(1) that the diagonal matrix element $\langle\Gamma|a_\alpha b_\beta|\Gamma\rangle = \delta_{\alpha\beta} \sum_{i=1} \delta_{i\alpha}$, where the sum over i is taken over all occupied orbitals in the m-particle state Γ. Placing this last equality into the trace equation, then taking the sum over β, and then breaking up the sum over α into a sum over orbitals in the first partition, denoted by α_1, and a sum over orbitals in the second

partition, denoted by α_2, we can write the configuration trace of O(1) as

$$\langle\langle O(1)\rangle\rangle_{S(m_1,m_2)} = \sum_{\Gamma\varepsilon S(m_1,m_2)} \sum_{\alpha_1} O_{\alpha_1\alpha_1} \sum_{i=1}^{m} \delta_{i\alpha_1} + \sum_{\alpha_2} O_{\alpha_2\alpha_2} \sum_{i=1}^{m} \delta_{i\alpha_2} \quad .$$

We will define the function

$$\Delta(\alpha_j;\Gamma) = \sum_{i=1}^{m} \delta_{i\alpha_j} \quad ,$$

which is defined as 1 (0) if α_j is (is not) an occupied orbital from the j-th partition in the state Γ, and then write

$$\langle\langle O(1)\rangle\rangle_{S(m_1,m_2)} = \sum_{\Gamma\varepsilon S(m_1,m_2)} \sum_{\alpha_1} O_{\alpha_1\alpha_1} \Delta(\alpha_1;\Gamma) + \sum_{\Gamma\varepsilon S(m_1,m_2)} \sum_{\alpha_2} O_{\alpha_2\alpha_2} \Delta(\alpha_2;\Gamma) \quad .$$

In the first term, the sum over Γ and the function $\Delta(\alpha_1;\Gamma)$ can be replaced (Appendix C) by a multiple occurrence factor

$$\left[\binom{N_1}{m_1}\binom{N_2}{m_2}\right]\left[\binom{m_1}{0}\binom{m_2}{0}\right]\Big/\left[\binom{N_1}{1}\binom{N_2}{0}\right] = \binom{N_1-1}{m_1-1}\binom{N_2}{m_2} \quad ,$$

where $\binom{N_1}{m_1}\binom{N_2}{m_2}$ is the number of m-particle states in the configuration space $S(\vec{m})$, $\binom{m_1}{1}\binom{m_2}{0}$ is the number of states with one particle in the first partition and no particles in the second partition that can be constructed from the single-particle states in Γ, and finally, $\binom{N_1}{1}\binom{N_2}{0}$ is the number of states with on particle in the first partition and no particle in the second partition that can be constructed

from the full set of N_1 and N_2 orbitals. Similarly, the sum over Γ and the function $\Delta(\alpha_2;\Gamma)$ can be replaced by

$$\left[\binom{N_1}{m_1}\binom{N_2}{m_2}\right]\left[\binom{m_1}{0}\binom{m_2}{1}\right]\Big/\left[\binom{N_1}{0}\binom{N_2}{1}\right] = \binom{N_1}{m_2}\binom{N_2-1}{m_2-1} \quad ,$$

and the configuration trace of O(1) becomes

$$\ll O(1)\gg_{S(m_1,m_2)} = \binom{N_1-1}{m_1-1}\binom{N_2}{m_2}\sum_{\alpha_1} O_{\alpha_1\alpha_1} + \binom{N_1}{m_1}\binom{N_2-1}{m_2-1}\sum_{\alpha_2} O_{\alpha_2\alpha_2} . \quad (3.37)$$

For the two-partitioned configuration trace of a two-body operator O(2), we write

$$\ll O(2)\gg_{S(m_1,m_2)} = \sum_{\Gamma\varepsilon S(m_1,m_2)} \sum_{\alpha\beta\gamma\delta} \langle O_{\alpha\beta\gamma\delta}\ \Gamma | a_\alpha a_\beta b_\gamma b_\delta | \Gamma\rangle \quad .$$

The development of this configuration trace is very similar to that of the scalar trace of O(2), which we derived earlier in this section. However, instead of summing over all α and β as we did in Eq. (3.18), we will now break the sum of single-particle states into sums over the two partitions, using the subscripts 1 and 2 to refer to the first and second partitions. Thus, we write the configuration trace as

$$\begin{aligned}\ll O(2)\gg_{S(m_1,m_2)} = \sum_{\Gamma\varepsilon S(m_1,m_2)} \Bigg(& \sum_{\alpha_1\beta_1} {}^2O_{\alpha_1\beta_1\beta_1\alpha_1}\ \Delta(\alpha_1,\beta_1;\Gamma) \\ & + \sum_{\alpha_1\beta_2} {}^2O_{\alpha_1\beta_2\beta_2\alpha_1}\ \Delta(\alpha_1,\beta_2;\Gamma) \\ & + \sum_{\alpha_2\beta_1} {}^2O_{\alpha_2\beta_1\beta_1\alpha_2}\ \Delta(\alpha_2,\beta_1;\Gamma) \\ & + \sum_{\alpha_2\beta_2} {}^2O_{\alpha_2\beta_2\beta_2\alpha_2}\ \Delta(\alpha_2,\beta_2;\Gamma) \Bigg) \end{aligned} \quad (3.38)$$

where $\Delta(\alpha_i,\beta_j;\Gamma)$ is defined as 1 if α_i and β_j are both occupied orbitals in Γ, and is zero otherwise. As we did in the previous examples for both scalar and configuration traces, we will replace (Appendix C) the sums over $\Gamma\varepsilon S(m_1,m_2)$ with the function $\Delta(\alpha_i,\beta_j;\Gamma)$ with the following multiple occurrence factors: in the first term in Eq. (3.38) the factor is

$$\left[\binom{N_1}{m_1}\binom{N_2}{m_2}\right]\left[\binom{m_1}{2}\binom{m_2}{0}\right]/\left[\binom{N_1}{2}\binom{N_2}{0}\right] = \binom{N_1-2}{m_1-2}\binom{N_2}{m_2} \quad ,$$

in the second and third terms the factor is

$$\left[\binom{N_1}{m_1}\binom{N_2}{m_2}\right]\left[\binom{m_1}{1}\binom{m_2}{1}\right]/\left[\binom{N_1}{1}\binom{N_2}{1}\right] = \binom{N_1-1}{m_1-1}\binom{N_2-1}{m_2-1} \quad ,$$

and in the last term the factor is

$$\left[\binom{N_1}{m_1}\binom{N_2}{m_2}\right]\left[\binom{m_1}{0}\binom{m_2}{2}\right]/\left[\binom{N_1}{0}\binom{N_2}{2}\right] = \binom{N_1}{m_1}\binom{N_2-2}{m_2-2} \quad .$$

Thus, the configuration trace for the operator O(2) can be written as

$$\begin{aligned}\langle\langle O(2)\rangle\rangle_{S(m_1,m_2)} = {} & \binom{N_1-2}{m_1-2}\binom{N_2}{m_2} \sum_{\alpha_1\beta_1} {}^2O_{\alpha_1\beta_1\beta_1\alpha_1} \\ & + \binom{N_1-1}{m_1-1}\binom{N_2-1}{m_2-1} \sum_{\alpha_1\beta_2} {}^2O_{\alpha_1\beta_2\beta_2\alpha_1} \\ & + \binom{N_1-1}{m_1-1}\binom{N_2-1}{m_2-1} \sum_{\alpha_2\beta_1} {}^2O_{\alpha_2\beta_1\beta_1\alpha_2} \\ & + \binom{N_1}{m_2}\binom{N_2-2}{m_2-2} \sum_{\alpha_2\beta_2} {}^2O_{\alpha_2\beta_2\beta_2\alpha_2} \quad . \end{aligned} \tag{3.39}$$

For the two-partitioned configuration trace of the square of the one-body operator $O^2(1)$, we begin by writing the operator as

$$O^2(1) = \bar{O}(1) + \bar{O}(2) \quad ,$$

where the operators $\bar{O}(1)$ and $\bar{O}(2)$ are defined in Eq. (3.20). Then the configuration trace of $O^2(1)$ can be written as

$$\langle\langle O^2(1)\rangle\rangle_{S(m_1,m_2)} = \langle\langle \bar{O}(1)\rangle\rangle_{S(m_1,m_2)} + \langle\langle \bar{O}(2)\rangle\rangle_{S(m_1,m_2)} \quad . \tag{3.40}$$

The first term in Eq. (3.40) is determined in the same way as the configuration trace for the one-body operator O(1), which we calculated in Eq. (3.37). Therefore, for the first term in Eq. (3.40) we can write

$$\begin{aligned}\langle\langle \bar{O}(1)\rangle\rangle_{S(m_1,m_2)} &= \binom{N_1-1}{m_1-1}\binom{N_2}{m_2} \sum_{\alpha_1} \bar{O}_{\alpha_1\alpha_1} + \binom{N_1}{m_1}\binom{N_2-1}{m_2-1} \sum_{\alpha_2} \bar{O}_{\alpha_2\alpha_2} \\ &= \binom{N_1-1}{m_1-1}\binom{N_2}{m_2}\left(\sum_{\alpha_1\beta_1} O_{\alpha_1\beta_1}O_{\beta_1\alpha_1} + \sum_{\alpha_1\beta_2} O_{\alpha_1\beta_2}O_{\beta_2\alpha_1} \right) \\ &\quad + \binom{N_1}{m_1}\binom{N_2-1}{m_2-1}\left(\sum_{\alpha_2\beta_1} O_{\alpha_2\beta_1}O_{\beta_1\alpha_2} + \sum_{\alpha_2\beta_2} O_{\alpha_2\beta_2}O_{\beta_2\alpha_2} \right).\end{aligned} \tag{3.41}$$

The second term in Eq. (3.40) is determined in the same manner as the configuration trace for the two-body operator O(2), except that now the coefficients do not contain the antisymmetrization property, that is, $\bar{O}_{\alpha\beta\beta\alpha} \neq -\bar{O}_{\alpha\beta\alpha\beta}$. If we replace $2\,O_{\alpha_i\beta_j\beta_j\alpha_i}$ by $(O_{\alpha_i\beta_j}O_{\alpha_i\beta_j} - O_{\alpha_i\beta_j}O_{\beta_j\alpha_i})$ in Eq. (3.39), where i, j = 1, 2, we then can write

$$\langle\langle\bar{O}(2)\rangle\rangle_{S(m_1,m_2)} = \binom{N_1-2}{m_1-2}\binom{N_2}{m_2} \sum_{\alpha_1\beta_1} (O_{\alpha_1\alpha_1}O_{\beta_1\beta_1} - O_{\alpha_1\beta_1}O_{\beta_1\alpha_1})$$

$$+ \binom{N_1-1}{m_1-1}\binom{N_2-1}{m_2-1} \sum_{\alpha_1\beta_2} (O_{\alpha_1\alpha_1}O_{\beta_2\beta_2} - O_{\alpha_1\beta_2}O_{\beta_2\alpha_1})$$

$$+ \binom{N_1-1}{m_1-1}\binom{N_2-1}{m_2-1} \sum_{\alpha_2\beta_1} (O_{\alpha_2\alpha_2}O_{\beta_1\beta_1} - O_{\alpha_2\beta_1}O_{\beta_1\alpha_2})$$

$$+ \binom{N_1}{m_1}\binom{N_2-2}{m_2-2} \sum_{\alpha_2\beta_2} (O_{\alpha_2\alpha_2}O_{\beta_2\beta_2} - O_{\alpha_2\beta_2}O_{\beta_2\alpha_2}) \quad . \tag{3.42}$$

Now, we can use the identity $\binom{N-J}{m-J} - \binom{N-J-1}{m-J-1} = \binom{N-J-1}{m-J}$ for J = 1, 2 to combine terms with the same subscripts on the coefficients when we place Eqs. (3.41) and (3.42) into Eq. (3.40). Finally, we can write the configuration trace for $O^2(1)$ as

$$\langle\langle O^2(1)\rangle\rangle_{S(m_1,m_2)} = \binom{N_1-2}{m_1-1}\binom{N_2}{m_2} \sum_{\alpha_1\beta_1} O_{\alpha_1\beta_1}O_{\beta_1\alpha_1}$$

$$+ \binom{N_1-2}{m_1-2}\binom{N_2}{m_2} \sum_{\alpha_1\beta_1} O_{\alpha_1\alpha_1}O_{\beta_1\beta_1}$$

$$+ \binom{N_1-1}{m_1-1}\binom{N_2-1}{m_2} \sum_{\alpha_1\beta_2} O_{\alpha_1\beta_2}O_{\beta_2\alpha_1}$$

$$+ \binom{N_1-1}{m_1-1}\binom{N_2-1}{m_2-1} \sum_{\alpha_1\beta_2} O_{\alpha_1\alpha_1}O_{\beta_2\beta_2}$$

$$+ \binom{N_1-1}{m_1}\binom{N_2-1}{m_2-1} \sum_{\alpha_2\beta_1} O_{\alpha_2\beta_1}O_{\beta_1\alpha_2}$$

$$+ \binom{N_1-1}{m_1-1}\binom{N_2-1}{m_2-1} \sum_{\alpha_2\beta_1} {}^{0}\alpha_2\alpha_2\,{}^{0}\beta_1\beta_1$$

$$+ \binom{N_1}{m_1}\binom{N_2-2}{m_1-1} \sum_{\alpha_2\beta_2} {}^{0}\alpha_2\beta_2\,{}^{0}\beta_2\alpha_2$$

$$+ \binom{N_1}{m_1}\binom{N_2-2}{m_2-2} \sum_{\alpha_2\beta_2} {}^{0}\alpha_2\alpha_2\,{}^{0}\beta_2\beta_2 \quad . \tag{3.43}$$

For a k-body operator O(k), we see in Appendix C that the configuration trace can be written as

$$\langle\langle O(k)\rangle\rangle_{S(\vec{m})} = \sum_{\vec{k}} \binom{N_1-k_1}{N_2-k_2} \cdots \binom{N_\ell-k_\ell}{m_\ell-k_\ell} \langle\langle O(k)\rangle\rangle_{S(\vec{k})} \quad , \tag{3.44}$$

where $\vec{k} = (k_1, k_2, \ldots, k_\ell)$ such that $k_1 \le m_1, \ldots, k_\ell \le m_\ell$, and $k_1+k_2+ \ldots + k_\ell = k$, and the sum is taken over all k which satisfy these conditions.

For a product of operators K, which is defined in Eq. (3.26), the redefinition given in Eq. (3.27) will allow us to write the configuration trace of K as

$$\langle\langle K\rangle\rangle_{S(\vec{m})} = \sum_{k=0}^{k'} \langle\langle O(k)\rangle\rangle_{S(\vec{m})} \quad , \tag{3.45}$$

where k' is the number of creation operators (and also the number of destruction operators) in the product K, and the configuration trace $\langle\langle O(k)\rangle\rangle_{S(\vec{m})}$ is expressed in Eq. (3.44).

Both the k-body traces used to calculate the scalar trace of K in Eq. (3.28) and the $\vec{k}$ traces used to calculate the configuration trace of K in Eq. (3.45) are difficult to calculate except in very simple cases. A configuration trace reduction formula has been developed (18,19), which reduces to Eq. (3.29) for the case where $\vec{m} = (m)$, and it is useful for computing complicated products of operators. We will express the configuration trace as

$$\langle\langle K \rangle\rangle_{S(\vec{m})} = \sum_{\vec{k}} \sum_{\vec{t}} \binom{N_1-k_1}{m_1-t_1} \cdots \binom{N_\ell-k_\ell}{m_\ell-t_\ell} D^{\vec{k}}_{\vec{t}}(K) \quad , \tag{3.46}$$

where the sum over $\vec{k} = (k_1, \ldots, k_\ell)$ is restricted to those values such that $k_1 + \ldots + k_\ell = k$, which is the number of creation operators (also the number of destruction operators) in the product K. Also, the sum over $t = (t_1, \ldots, t_\ell)$ is restricted to those values such that $0 \leq t_i \leq$ smaller (k_i, m_k), $i = 1, \ldots, \ell$. The configuration basic diagrams $D^{\vec{k}}_{\vec{t}}(K)$ are determined by taking all possible full contractions between the k creation and k destruction operators such that k_i contractions are restricted to single particle labels in the i-th partition and t_i of these contractions are left contractions where the creation operator lies to the left of the destruction operator with which it is contracted. In addition, each fully contracted term will have a phase factor of +1 or -1 depending upon whether an even or odd (respectively) number of permutations of the operators is required to bring each of the contracted pairs together.

In determining the configuration basic diagram $D^{\vec{k}}_{\vec{t}}$, one can first determine the scalar basic diagram D^{k}_{t}, where $t_1 + \ldots + t_\ell = t$, and then restrict the single-particle labels to the partitions appropriate to satisfy the configuration basic diagram.

For the case where K = O(1), and $\vec{m} = (m_1, m_2)$, we can apply Eq. (3.46) so that

$$\langle\langle O(1)\rangle\rangle_{S(\vec{m})} = \binom{N_1-1}{m_1-1}\binom{N_2}{m_2} D^{1,0}_{1,0} + \binom{N_1}{m_1}\binom{N_2-1}{m_2-1} D^{0,1}_{0,1} \quad ,$$

and since there is no right contraction there will be no terms where $t_1 < k_1$ or $t_2 < k_2$. We learned earlier in this section that $D^{1}_{1}(O(1)) = \sum_{\alpha} O_{\alpha\alpha}$, and from this we can trivially write

$$D^{1,0}_{1,0}(O(1)) = \sum_{\alpha_1} O_{\alpha_1\alpha_1} \quad ,$$

and

$$D^{0,1}_{0,1}(O(1)) = \sum_{\alpha_2} O_{\alpha_2\alpha_2} \quad ,$$

so that

$$\langle\langle O(1)\rangle\rangle_{S(\vec{m})} = \binom{N_1-1}{m_1-1}\binom{N_2}{m_2} \sum_{\alpha_1} O_{\alpha_1\alpha_1} + \binom{N_1}{m_1}\binom{N_2-1}{m_2-1} \sum_{\alpha_2} O_{\alpha_2\alpha_2} \quad .$$

The configuration trace for O(1) as derived in this way equals that which was found by using Wick's theorem, as is evidenced by comparing this result with Eq. (3.37).

For the case where $K = 0^2(1)$, one set of contractions, $\overbrace{a_1^\dagger b_2}\overbrace{a_3^\dagger b_4} = +\delta_{12}\delta_{34}$, will have two left contractions, and the other set, i.e., $\overbrace{a_1^\dagger b_2 a_3^\dagger b_4} = +\delta_{14}\delta_{32}$, will have one left contraction.

The scalar basic diagram for the first set of contractions will be

$$D_2^2 = \sum_{\alpha\beta} O_{\alpha\alpha} O_{\beta\beta} \quad .$$

For the two-partition configuration, three configuration basic diagrams will be related to this scalar basic diagram:

$$\begin{aligned} D_{1,1}^{1,1} &= \sum_{\alpha_1\beta_2} O_{\alpha_1\alpha_1} O_{\beta_2\beta_2} + \sum_{\alpha_2\beta_1} O_{\alpha_2\alpha_2} O_{\beta_1\beta_1} \\ &= 2 \sum_{\alpha_1\beta_2} O_{\alpha_1\alpha_1} O_{\beta_2\beta_2} \quad , \end{aligned} \tag{3.47}$$

$$D_{2,0}^{2,0} = \sum_{\alpha_1\beta_1} O_{\alpha_1\alpha_1} O_{\beta_1\beta_1} \quad ,$$

and

$$D_{0,2}^{0,2} = \sum_{\alpha_2\beta_2} O_{\alpha_2\alpha_2} O_{\beta_2\beta_2} \quad .$$

The scalar basic diagram for the set of contractions where one is a left contraction is

$$D_1^2 = \sum_{\alpha\beta} O_{\alpha\beta} O_{\beta\alpha} \quad .$$

There will be four configuration basic diagrams related to this last diagram:

$$D^{1,1}_{1,0} = \sum_{\alpha_1\beta_2} O_{\alpha_1\beta_2} O_{\beta_2\alpha_1} \quad ,$$

$$D^{1,1}_{0,1} = \sum_{\alpha_2\beta_1} O_{\alpha_2\beta_1} O_{\beta_1\alpha_2} \quad , \tag{3.48}$$

$$D^{2,0}_{1,0} = \sum_{\alpha_1\beta_1} O_{\alpha_1\beta_1} O_{\beta_1\alpha_1} \quad ,$$

and

$$D^{0,2}_{0,1} = \sum_{\alpha_2\beta_2} O_{\alpha_2\beta_2} O_{\beta_2\alpha_2} \quad .$$

We now can place these configuration basic diagrams in Eqs. (3.47) and (3.48) into the configuration trace formula, Eq. (3.46), and find the configuration trace for $O^2(1)$ to be

$$\begin{aligned} \langle\langle O^2(1)\rangle\rangle_{S(\vec{m})} = {} & 2\binom{N_1-1}{m_1-1}\binom{N_2-1}{m_2-1} \sum_{\alpha_1\beta_2} O_{\alpha_1\alpha_1} O_{\beta_2\beta_2} \\ & + \binom{N_1-2}{m_1-2}\binom{N_2}{m_2} \sum_{\alpha_1\beta_1} O_{\alpha_1\alpha_1} O_{\beta_1\beta_1} \\ & + \binom{N_1}{m_1}\binom{N_2-2}{m_2-2} \sum_{\alpha_2\beta_2} O_{\alpha_2\alpha_2} O_{\beta_2\beta_2} \\ & + \binom{N_1-1}{m_1-1}\binom{N_2-1}{m_2} \sum_{\alpha_1\beta_2} O_{\alpha_1\beta_2} O_{\beta_2\alpha_1} \\ & + \binom{N_1-1}{m_1}\binom{N_2-1}{m_2-1} \sum_{\alpha_2\beta_1} O_{\alpha_2\beta_1} O_{\beta_1\alpha_2} \end{aligned}$$

$$+ \binom{N_1-2}{m_1-1}\binom{N_2}{m_2} \sum_{\alpha_1\beta_1} O_{\alpha_1\beta_1} O_{\beta_1\alpha_1}$$

$$+ \binom{N_1}{m_1}\binom{N_2-2}{m_2-1} \sum_{\alpha_2\beta_2} O_{\alpha_2\beta_2} O_{\beta_2\alpha_2} \quad .$$

This last result agrees with the result in Eq. (3.43) where we decomposed $O^2(1)$ into $\bar{O}(1) + \bar{O}(2)$ and then applied Wick's theorem.

For the example where $K = O^2(2)$, there are three scalar basic diagrams, as was shown earlier in this section. For a two-partition configuration, five configuration basic diagrams can be constructed from the scalar basic diagram D^4_4:

$$D^{4,0}_{4,0} = 4\Big(\sum_{\alpha_1\beta_1} O_{\alpha_1\beta_1\beta_1\alpha_1} \Big)^2 \quad ,$$

$$D^{3,1}_{3,1} = 16 \sum_{\alpha_1\beta_2} O_{\alpha_1\beta_2\beta_2\alpha_1} \sum_{\alpha_1\beta_1} O_{\alpha_1\beta_1\beta_1\alpha_1} \quad ,$$

$$D^{2,2}_{2,2} = 16\Big(\sum_{\alpha_1\beta_2} O_{\alpha_1\beta_2\beta_2\alpha_1} \Big)^2 + 8 \sum_{\alpha_1\beta_1} O_{\alpha_1\beta_1\beta_1\alpha_1} \sum_{\alpha_2\beta_2} O_{\alpha_2\beta_2\beta_2\alpha_2} \quad , \quad (3.49a)$$

$$D^{1,3}_{1,3} = 16 \sum_{\alpha_1\beta_2} O_{\alpha_1\beta_2\beta_2\alpha_1} \sum_{\alpha_2\beta_2} O_{\alpha_2\beta_2\beta_2\alpha_2} \quad ,$$

and

$$D^{0,4}_{0,4} = 4\Big(\sum_{\alpha_2\beta_2} O_{\alpha_2\beta_2\beta_2\alpha_2} \Big)^2 \quad .$$

From the scalar basic diagram D^4_3, we can construct eight configuration basic diagrams:

$$D^{4,0}_{3,0} = 16 \sum_{\substack{\alpha_1\beta_1 \\ \gamma_1\delta_1}} {}^{0}\alpha_1\beta_1\beta_1\gamma_1\,{}^{0}\gamma_1\delta_1\delta_1\alpha_1 \quad ,$$

$$D^{3,1}_{3,0} = 16 \sum_{\substack{\alpha_1\beta_1 \\ \gamma_2\delta_1}} {}^{0}\alpha_1\beta_1\beta_1\gamma_2\,{}^{0}\gamma_2\delta_1\delta_1\alpha_1 \quad ,$$

$$D^{3,1}_{2,1} = 32 \sum_{\substack{\alpha_1\beta_2 \\ \gamma_1\delta_1}} {}^{0}\alpha_1\beta_2\beta_2\gamma_1\,{}^{0}\gamma_1\delta_1\delta_1\alpha_1 + 16 \sum_{\substack{\alpha_2\beta_1 \\ \gamma_1\delta_1}} {}^{0}\alpha_2\beta_1\beta_1\gamma_1\,{}^{0}\gamma_1\delta_1\delta_1\alpha_2 \quad ,$$

$$D^{2,2}_{2,1} = 32 \sum_{\substack{\alpha_1\beta_1 \\ \gamma_2\delta_2}} {}^{0}\alpha_1\beta_1\beta_1\gamma_2\,{}^{0}\gamma_2\delta_2\delta_2\alpha_1 + 16 \sum_{\substack{\alpha_2\beta_1 \\ \gamma_2\delta_1}} {}^{0}\alpha_2\beta_1\beta_1\gamma_2\,{}^{0}\gamma_2\delta_1\delta_1\alpha_2 \quad , \tag{3.49b}$$

$$D^{2,2}_{1,2} = 32 \sum_{\substack{\alpha_2\beta_2 \\ \gamma_1\delta_1}} {}^{0}\alpha_2\beta_2\beta_2\gamma_1\,{}^{0}\gamma_1\delta_1\delta_1\alpha_2 + 16 \sum_{\substack{\alpha_1\beta_2 \\ \gamma_1\delta_2}} {}^{0}\alpha_1\beta_2\beta_2\gamma_1\,{}^{0}\gamma_1\delta_2\delta_2\alpha_1 \quad ,$$

$$D^{1,3}_{1,2} = 32 \sum_{\substack{\alpha_2\beta_1 \\ \gamma_2\delta_2}} {}^{0}\alpha_2\beta_1\beta_1\gamma_2\,{}^{0}\gamma_2\delta_2\delta_2\alpha_2 + 16 \sum_{\substack{\alpha_1\beta_2 \\ \gamma_2\delta_2}} {}^{0}\alpha_1\beta_2\beta_2\gamma_2\,{}^{0}\gamma_2\delta_2\delta_2\alpha_1 \quad ,$$

$$D^{1,3}_{0,3} = 16 \sum_{\substack{\alpha_2\beta_2 \\ \gamma_1\delta_2}} {}^{0}\alpha_2\beta_2\beta_2\gamma_1\,{}^{0}\gamma_1\delta_2\delta_2\alpha_2 \quad ,$$

and

$$D^{0,4}_{0,3} = 16 \sum_{\substack{\alpha_2\beta_2 \\ \gamma_2\delta_2}} {}^{0}\alpha_2\beta_2\beta_2\gamma_2\,{}^{0}\gamma_2\delta_2\delta_2\alpha_2 \quad .$$

Finally, from the scalar basic diagram D^4_2, we can construct nine configuration basic diagrams:

$$D^{4,0}_{2,0} = 4 \sum_{\substack{\alpha_1\beta_1 \\ \gamma_1\delta_1}} O^2_{\alpha_1\beta_1\gamma_1\delta_1} ,$$

$$D^{3,1}_{2,0} = 8 \sum_{\substack{\alpha_1\beta_1 \\ \gamma_1\delta_2}} O^2_{\alpha_1\beta_1\gamma_1\delta_2} ,$$

$$D^{3,1}_{1,1} = 8 \sum_{\substack{\alpha_2\beta_1 \\ \gamma_1\delta_1}} O^2_{\alpha_2\beta_1\gamma_1\delta_1} ,$$

$$D^{2,2}_{2,0} = 4 \sum_{\substack{\alpha_1\beta_1 \\ \gamma_2\delta_2}} O^2_{\alpha_1\beta_1\gamma_2\delta_2} ,$$

$$D^{2,2}_{1,1} = 16 \sum_{\substack{\alpha_1\beta_2 \\ \gamma_2\delta_1}} O^2_{\alpha_1\beta_2\gamma_2\delta_1} , \qquad (3.49c)$$

$$D^{2,2}_{0,2} = 4 \sum_{\substack{\alpha_2\beta_2 \\ \gamma_1\delta_1}} O^2_{\alpha_2\beta_2\gamma_1\delta_1} ,$$

$$D^{1,3}_{1,1} = 8 \sum_{\substack{\alpha_1\beta_2 \\ \gamma_2\delta_2}} O^2_{\alpha_1\beta_2\gamma_2\delta_2} ,$$

$$D^{1,3}_{0,2} = 4 \sum_{\substack{\alpha_2\beta_2 \\ \gamma_2\delta_1}} O^2_{\alpha_2\beta_2\gamma_2\delta_1} ,$$

and

$$D^{0,4}_{0,2} = 4 \sum_{\substack{\alpha_2\beta_2 \\ \gamma_2\delta_2}} O^2_{\alpha_2\beta_2\gamma_2\delta_2} \quad .$$

C. Polynomial Expansions for Expectation Values

We are interested in calculating the expectation values of a general operator K as a function of the discrete energy E' of the eigenvector $|E'\rangle$ of a many-body Hamiltonian H, where we use the trace techniques that we have discussed in the previous section.

We will begin by expanding the expectation value $\langle E'|K|E'\rangle$ in terms of a complete set of orthogonal polynomials in E', $\{P_N(E'): N=0,\infty\}$, that is

$$\langle E'|K|E'\rangle = \sum_{N=0}^{\infty} C_N P_N(E') \quad . \tag{3.50}$$

(The orthogonal polynomials are briefly reviewed in Appendix D.)

Now, for a given Hamiltonian with a finite number of states, the distribution of eigenenergies is discrete and the number of eigenstates d will possibly be greater than the number of energy values q because of degeneracies. Now, we will assume the existence of a continuous density of states function $\rho(E)$, whose first 2q moments are equal to the first 2q moments of the discrete distribution of eigenenergies of the Hamiltonian H, that is

$$\int_L E^n \rho(E)\, dE = \sum_{A=1}^{d} \langle A|H^n|A\rangle/d$$

$$= \langle H^n\rangle \quad , \quad 0 \le n \le 2q-1 \quad , \tag{3.51}$$

where the continuous energy interval L includes the set of discrete eigenvalues $\{E_A: \ A = 1,d\}$. Then, as discussed in Appendix D, the q orthogonal polynomials defined in terms of the discrete set of energy values $\{E_A: \ A = 1,d\}$ will equal the first q orthogonal polynomials defined in terms of the continuous density of states function $\rho(E)$ defined over the energy interval L. Taking the polynomials of $\rho(E)$ to be the polynomials $P_N(E)$ used in the expansion Eq. (3.50), we then can use the discrete orthonormality relation

$$\langle P_N(H) \ P_M(H) \rangle \ = \ \delta_{NM} \quad , \quad N, M = 0, q-1$$

to solve for the first q coefficients, that is

$$\langle E'|K|E' \rangle \ = \ \sum_{N=0}^{q-1} \langle K \ P_N(H) \rangle P_N(E') + O(P_q(E')) \quad . \qquad (3.52)$$

We will be working with a finite Hamiltonian whose number of energy levels q is very large, but because the moments of H are too difficult to calculate if they are greater than two, we will be able to use only the first few terms in the expansion Eq. (3.52). We hope for rapid convergence with the lowest terms in that expansion.

Also, the eigenenergies $\{E_A: \ A = 1,d\}$ are expected to be so close that they are almost continuous, and, since the polynomials $P_N(E)$ exist for values of E other than the discrete eigenvalues E' of H, we will consider the right hand side of Eq. (3.52) to be continuous in E, and write

$$K(E) = \sum_{N=0}^{q-1} \langle K\, P_N(H) \rangle P_N(E) + O(P_q(E)) \tag{3.53}$$

for the continuous expectation value of the operator K.

IV. FORMULATION FOR RADIAL MOMENTS

In this chapter we develop the formulas needed to calculate the expectation value of the radial moments of the one-body density.

In Section A, we will define the radial moment operator and write the truncated expectation value expansion with scalar moments.

In Section B we will discuss how to find the expectation value for states with good isospin.

In the last section we will list all of the configuration diagrams that are involved in calculating the expectation values of the radial moment operator with good isospin.

A. Calculation of Radial Moments

We will use the techniques discussed in Chapter III to calculate the expectation value of the k-th power of the radial coordinate r, using the effective nuclear many-body Hamiltonian discussed in Chapter II.

In the operator representation (Eq. (2.32)) the p-th power of the radial coordinate has the one-body form $R^{(k)}$ given

$$R^{(k)} = \sum_{\alpha\beta} R^{(k)}_{\alpha\beta} \, a_\alpha \, b_\beta \quad , \tag{4.1}$$

where $\alpha = (n_\alpha, \ell_\alpha, j_{z\alpha}, j_\alpha)$. The coefficient $R^{(k)}_{\alpha\beta}$ is the one-body matrix element

$$R^{(k)}_{\alpha\beta} = \langle \bar{\alpha} | r^k | \bar{\beta} \rangle$$

$$= \int_0^\infty R^*_{\bar{\alpha}}(r)\ r^k\ R_{\bar{\beta}}(r)\ dr \quad , \tag{4.2}$$

where $\bar{\alpha} = (n_\alpha, \ell_\alpha, j_\alpha)$. The calculation of these coefficients using the spherical harmonic oscillator single-particle wavefunctions is discussed in Appendix E.

The expectation value of the radial operator $R^{(k)}$ is found by applying the expansion in orthogonal polynomials (Eq. (3.53)) so that

$$R^{(k)}(E) = \sum_{N=0}^{q-1} \langle R^{(k)}\ P_N(H)\rangle P_N(E) + O(P_q(E)) \quad . \tag{4.3}$$

We will be able to calculate only the first three moments of the Hamiltonian H, so that we can carry the expansion in Eq. (4.3) only through N = 1, that is

$$\begin{aligned} R^{(k)}(E) &\approx \langle R^{(k)}\ P_0(H)\rangle P_0(E) + \langle R^{(k)}\ P_1(H)\rangle P_1(E) \\ &= \langle R^{(k)}\rangle + \frac{(\langle R^{(k)}H\rangle - \langle R^{(k)}\rangle\langle H\rangle)(E - \langle H\rangle)}{(\langle H^2\rangle - \langle H\rangle^2)} \quad , \end{aligned} \tag{4.4}$$

where the first two orthogonal polynomials are given in Eq. (.4).

The trace reduction formulas for the scalar moments $\langle R^{(k)}\rangle$, $\langle H\rangle$, and $\langle H^2\rangle$ are given in Eqs. (3.16), (3.19) and (3.32a), respectively. For the trace reduction formula of the scalar moment $\langle R^{(k)}H\rangle$ which contains the product of a one- and two-body operator, we can apply Eq. (3.29) and write

$$\langle R^{(k)}{}_H\rangle = \binom{N}{m}^{-1} \left[\binom{N-3}{m-3} D_3^3(R^{(k)}H) + \binom{N-3}{m-2} D_2^3(R^{(k)}H)\right] \quad , \tag{4.5a}$$

where the basic diagrams are

$$D_3^3(R^{(k)}H) = 2 \sum_{\alpha\beta\gamma} R^{(k)}_{\alpha\alpha} H_{\beta\gamma\gamma\beta} \quad , \tag{4.5b}$$

and

$$D_2^3(R^{(k)}H) = 4 \sum_{\alpha\beta\gamma} R^{(k)}_{\alpha\beta} H_{\beta\gamma\gamma\alpha} \quad . \tag{4.5c}$$

From Eq. (2.38) we see that the two-body matrix elements of the Hamiltonian are written as

$$H_{\alpha\beta\gamma\delta} = -\frac{1}{4} {}_{s.d.}\langle\alpha\beta|H|\gamma\delta\rangle_{s.d.} \quad , \tag{4.6}$$

which is discussed in Chapter II.

B. Expectation Values with Good Isospin

If the eigenstates of the Hamiltonian H are also eigenstates of the square of the total isospin operator T^2, as well as eigenstate of the operator for the z component of isospin T_z, then we will be interested in finding the expectation value of the radial moments for a given total isospin quantum value t.

We begin by assuming the existence of a continuous density of states function $\rho_t(E)$ where all of the states in the distribution have a total isospin value t, with the z component isospin quantum value also equal to t. Then, the same reasoning that was used in Section C of the previous chapter can be applied to write the polynomial expansion for the expectation value of radial moments as

$$R_t^{(k)}(E) \approx \sum_{N=0}^{q-1} \langle R^{(k)} \; P_N^t(H) \rangle_{S(m,t)} \; P_N^t(E) \quad , \tag{4.7}$$

where S(m,t) denotes the set of eigenstates of the m-particle finite model space Hamiltonian with total isospin and z component equal to t. The set of polynomials $\{P_N^t(E)\}_{N=0}^{q-1}$ are orthogonal with respect to the discrete distribution of q energy levels of the states in S(m,t), similar to what is shown in Eq. (3.51).

The shell model states which are in the set S'(m) Eq. (3.12) are not eigenstates of the total isospin operator T^2, but they are eigenstates of the z component of the total isospin operator T_z. Then, by Eq. (3.11), we can write, for an operator K, the trace relations

$$\langle\langle K \rangle\rangle_{S'(m,t_z)} = \langle\langle K \rangle\rangle_{S(m,t_z)} \quad , \tag{4.8}$$

where $S'(m,t_z)$ is the subset of shell model basis states which have the z component of the total isospin value of t_z, and $S(m,t_z)$ is the subset of all eigenstates of the Hamiltonian H which have the z component of the total isospin value equal to t_z.

Now, if the matrix elements in the moment $\langle K \rangle_{S(m,t)}$ are <u>independent</u> of the z component of total isospin, we find that the following relationship holds:

$$d(t)\langle K \rangle_{S(m,t)} = d(t_z)\langle K \rangle_{S(m,t_z)} - d(t_z + 1)\langle K \rangle_{S(m,t_z + 1)} \; , \tag{4.9}$$

where d(t) is the dimensionality of states in S(m,t), and similarly for $d(t_z)$ and $d(t_z + 1)$. Then, by Eq. (4.8) we have

$$d(t)\langle K\rangle_{S(m,t)} = d(t_z)\langle K\rangle_{S'(m,t_z)} - d(t_z + 1)\langle K\rangle_{S'(m,t_z+1)} \quad . \tag{4.10}$$

(Note that if a Coulomb part is included in the Hamiltonian then the z component of total isospin, but not the total isospin, is a good quantum number. In that case we would work with Eq. (4.8).)

Now, by letting $K \equiv 1$, we find that Eq. (4.10) becomes

$$d(t) = d(t_z) - d(t_z + 1) \quad . \tag{4.11}$$

With the above approximations we can calculate traces of fixed isospin $T = t_z = t$.

The x component of the total isospin value t_z of a shell model state of m-particles is equal to the sum of the z-components of isospin of the individual particles, that is

$$t_z = \sum_{i=1}^{m} (t_z)_i \quad , \tag{4.12}$$

where $(t_z)_i$ is the isospin of the i-th particle. If we use the convention that the isospin of a proton (neutron) is $+\frac{1}{2}$ $(-\frac{1}{2})$, then Eq. (4.12) becomes

$$t_z = \frac{m_p - m_n}{2} \quad , \tag{4.13}$$

where $m_p (m_n)$ is the number of protons (neutrons).

Because the total number of particles $m = m_p + m_n$ is also a good quantum number for the states in the subset $S'(m,t_z)$, the following connection can be made with configuration traces:

$$\langle K \rangle_{S'(m,t_z)} = \langle K \rangle_{S'(\vec{m})} \quad , \tag{4.14a}$$

where $\vec{m} = (m_p, m_n)$. Then the dimensionalities are given as

$$d(t_z) = \binom{N_p}{m_p} \binom{N_n}{m_n} \quad , \tag{4.14b}$$

$$d(t_z + 1) = \binom{N_p}{m_p+1} \binom{N_n}{m_n-1} \quad , \tag{4.14c}$$

and

$$d(t) = \binom{N_p}{m_p} \binom{N_n}{m_n} - \binom{N_p}{m_p+1} \binom{N_n}{m_n-1} \quad . \tag{4.14d}$$

The calculation of the configuration moments that will be used in Eq. (4.7) will require the one-body matrix elements of the radial moment operator, $\langle \alpha_p | r^k | \beta_p \rangle$ and $\langle \alpha_n | r^k | \beta_n \rangle$, where the subscripts p(n) denote proton (neutron) orbitals. Since the operator conserves isospin, the matrix elements $\langle \alpha_p | r^k | \beta_n \rangle = \langle \alpha_n | r^k | \beta_p \rangle = 0$, and, wehere we assume the same radial wavefunctions for neutron and proton orbitals, we have

$$\langle \alpha_p | r^k | \beta_p \rangle = \langle \alpha_n | r^k | \beta_n \rangle = \langle \alpha | r^k | \beta \rangle \quad . \tag{4.15}$$

The following two-body matrix elements will also be required in the calculation Eq. (4.7): $\langle \alpha_p \beta_p | H | \gamma_p \delta_p \rangle$, $\langle \alpha_n \beta_n | H | \gamma_n \delta_n \rangle$, and $\langle \alpha_p \beta_n | H | \gamma_p \delta_n \rangle$. The actual two-body matrix elements that will be used in this work are given in the coupled J - T representation (21) $\langle (\bar{\alpha}, \bar{\beta}) JT | H | (\bar{\gamma}, \bar{\delta}) JT \rangle$, where $\bar{\alpha} = (n_\alpha, \ell_\alpha, j_\alpha)$, and the two-particle states $|\alpha, \beta\rangle$ are coupled to total

spin $J = j_\alpha + j_\beta = j_\gamma + j_\delta$ and isospin $T = t_\alpha + t_\beta = t_\gamma + t_\delta$ using the Clebsch-Gordon expansion.

For coupled J matrix elements with proton and/or neutron orbitals, we can use the inverse Clebsch-Gordon expansion, summing over total isospin T, to write

$$U^J_{\bar{\alpha}\bar{\beta}\bar{\gamma}\bar{\delta}} = N^{-1}_{\bar{\alpha}\bar{\beta}} N^{-1}_{\bar{\gamma}\bar{\delta}} \langle(\bar{\alpha},\bar{\beta})J,\ T=1|H'|(\bar{\gamma},\bar{\delta})J,\ T=1\rangle \quad , \tag{4.16a}$$

for the proton-proton configuration, where H' is the Hamiltonian, possibly including the Coulomb potential (which means that the eigenstate then would not possess a good total isospin quantum number, but that the z component of isospin would be a good number), and $N_{\bar{\alpha}\bar{\beta}} = (1 + \delta_{\bar{\alpha}\bar{\beta}})^{-1/2}$ is a normalization factor. Similarly, for the neutron-neutron configuration we write

$$V^J_{\bar{\alpha}\bar{\beta}\bar{\gamma}\bar{\delta}} = N^{-1}_{\bar{\alpha}\bar{\beta}} N^{-1}_{\bar{\gamma}\bar{\delta}} \langle(\bar{\alpha},\bar{\beta})J,\ T=1|H|(\bar{\gamma},\bar{\delta})J,\ T=1\rangle \quad . \tag{4.16b}$$

Note that if the Coulomb interaction is not included, then H' = H and Eq. (4.16a) equals Eq. (4.16b). Finally, for the proton-neutron configuration matrix element we write

$$W^J_{\bar{\alpha}\bar{\beta}\bar{\gamma}\bar{\delta}} = \frac{N^{-1}_{\bar{\alpha}\bar{\beta}} N^{-1}_{\bar{\gamma}\bar{\delta}}}{2} \left(\langle(\bar{\alpha},\bar{\beta})J,\ T=1|H|(\bar{\gamma},\bar{\delta})J,\ T=1\rangle + \langle(\bar{\alpha},\bar{\beta})J,\ T=0|H|(\bar{\gamma},\bar{\delta})J,\ T=0)\rangle\right) \quad . \tag{4.16c}$$

Thus we have all of the types of one- and two-body matrix elements that will be used in this work.

C. Configuration Diagrams

In this section we will present the diagrams for the operator traces that are used in the calculation of the expectation value $R_t^{(k)}(E)$.

The configuration diagrams used to calculate the trace of the operator $R^{(k)}$ are

$$D_{10}^{10}(R_p^{(k)}) = \sum_{\alpha} (2j_\alpha + 1)\langle\alpha|r^k|\alpha\rangle \quad ,$$

and

$$D_{01}^{01}(R_n^{(k)}) = D_{10}^{10}(R_p^{(k)}) \quad ,$$

where $\alpha = (n_\alpha, \ell_\alpha, j_\alpha)$.

The configuration diagrams used to calculate the trace of the Hamiltonian $\langle H\rangle_{S(m_p,m_n)}$ are

$$D_{20}^{20}(U) = \frac{1}{2} \sum_{\alpha,\beta,J} (2J + 1)\, U^J_{\alpha\beta\alpha\beta} \quad ,$$

$$D_{02}^{02}(V) = \frac{1}{2} \sum_{\alpha,\beta,J} (2J + 1)\, V^J_{\alpha\beta\alpha\beta} \quad ,$$

and

$$D_{11}^{11}(W) = \sum_{\alpha,\beta,J} (2J + 1)\, W^J_{\alpha\beta\alpha\beta} \quad .$$

The configuration diagrams used to calculate the trace of the product of the radial moment operator and the Hamiltonian $\langle R^{(k)}H\rangle_{S(m_p,m_n)}$ are

$$D^{30}_{30}(R^{(k)}_p U) = D^{10}_{10}(R^{(k)}_p)\, D^{20}_{20}(U) \quad ,$$

$$D^{21}_{21}(R^{(k)}_n U) = D^{10}_{10}R^{(k)}_p)\, D^{20}_{20}(U) \quad ,$$

$$D^{21}_{21}(R^{(k)}_p W) = D^{10}_{10}(R^{(k)}_p)\, D^{11}_{11}(W) \quad ,$$

$$D^{12}_{12}(R^{(k)}_p V) = D^{10}_{10}(R^{(k)}_p)\, D^{02}_{02}(V) \quad ,$$

$$D^{12}_{12}(R^{(k)}_n W) = D^{10}_{10}(R^{(k)}_p)\, D^{11}_{11}(W) \quad ,$$

$$D^{03}_{03}(R^{(k)}_n V) = D^{10}_{10}(R^{(k)}_p)\, D^{02}_{02}(V) \quad ,$$

$$D^{30}_{20}(R^{(k)}_p U) = \sum_{\alpha,\beta} \delta(j_\alpha, j_\beta)\langle\alpha|r^k|\beta\rangle \sum_{\gamma J} (2J+1) U^J_{\alpha\gamma\beta\gamma} \quad ,$$

$$D^{21}_{11}(R^{(k)}_p W) = \sum_{\alpha,\beta} \delta(j_\alpha, j_\beta)\langle\alpha|r^k|\beta\rangle \sum_{\gamma J} (2J+1) W^J_{\alpha\gamma\beta\gamma} \quad ,$$

$$D^{12}_{11}(R^{(k)}_n W) = D^{21}_{11}(R^{(k)}_p W) \quad ,$$

and

$$D^{03}_{02}(R^{(k)}_n V) = \sum_{\alpha,\beta} \delta(j_\alpha, j_\beta)\langle\alpha|r^k|\beta\rangle \sum_{\gamma J} (2J+1) V^J_{\alpha\gamma\beta\gamma} \quad ,$$

where $\delta(j_\alpha, j_\beta)$ is the Kronecker delta.

The configuration diagrams used to calculate the trace of the square of the Hamiltonian $\langle H^2\rangle_{S(m_p,m_n)}$ are

$$D_{20}^{40}(U^2) = \frac{1}{4} \sum_{\substack{\alpha,\beta,\gamma,\delta,\\ J}} (2J+1)\left(U^J_{\alpha\beta\gamma\delta}\right)^2 ,$$

$$D_{11}^{22}(W^2) = \sum_{\substack{\alpha,\beta,\gamma,\delta,\\ J}} (2J+1)\left(W^J_{\alpha\beta\gamma\delta}\right)^2 ,$$

$$D_{02}^{04}(V^2) = \frac{1}{4} \sum_{\substack{\alpha,\beta,\gamma,\delta,\\ J}} (2J+1)\left(V^J_{\alpha\beta\gamma\delta}\right)^2 ,$$

$$D_{30}^{40}(U^2) = \sum_{\alpha,\gamma} \frac{\delta(j_\alpha,j_\gamma)}{(2j_\alpha+1)}\left(\sum_{\beta,J} (2J+1)\, U^J_{\alpha\beta\gamma\beta}\right)^2 ,$$

$$D_{31}^{31}(UW) = \sum_{\alpha,\gamma} \frac{\delta(j_\alpha,j_\gamma)}{(2j_\alpha+1)}\left(\sum_{\beta,J} (2J+1) W^J_{\alpha\beta\gamma\beta}\right)\left(\sum_{\beta,J} (2J+1) U^J_{\alpha\beta\gamma\beta}\right),$$

$$D_{21}^{31}(WU) = D_{21}^{31}(UW) ,$$

$$D_{21}^{22}(W^2) = \sum_{\alpha,\gamma} \frac{\delta(j_\alpha,j_\gamma)}{(2j_\alpha+1)}\left(\sum_{\beta,J} (2J+1)\, W^J_{\alpha\beta\gamma\beta}\right)^2 ,$$

$$D_{12}^{22}(W^2) = D_{21}^{22}(W^2) ,$$

$$D_{12}^{13}(WV) = \sum_{\alpha,\gamma} \frac{\delta(j_\alpha,j_\gamma)}{(2j_\alpha+1)}\left(\sum_{\beta,J} (2J+1)\, W^J_{\alpha\beta\gamma\beta}\right)\left(\sum_{\beta,J} (2J+1)\, V^J_{\alpha\beta\gamma\beta}\right) ,$$

$$D_{12}^{13}(VW) = D_{12}^{13}(WV) ,$$

$$D_{03}^{04}(V^2) = \sum_{\alpha,\gamma} \frac{\delta(j_\alpha,j_\gamma)}{(2j_\alpha+1)}\left(\sum_{\beta,J} (2J+1)\, V^J_{\alpha\beta\gamma\beta}\right)^2 ,$$

$$D_{40}^{40}(U^2) = \left(D_{20}^{20}(W) \right)^2 ,$$

$$D_{31}^{31}(WU) = D_{11}^{11}(W)\ D_{20}^{20}(U) ,$$

$$D_{31}^{31}(UW) = D_{31}^{31}(WU) ,$$

$$D_{22}^{22}(UV) = D_{20}^{20}(U)\ D_{02}^{02}(V) ,$$

$$D_{22}^{22}(W^2) = \left(D_{11}^{11}(W) \right)^2 ,$$

$$D_{22}^{22}(VU) = D_{22}^{22}(UV) ,$$

$$D_{13}^{13}(WV) = D_{11}^{11}(W)\ D_{02}^{02}(V) ,$$

$$D_{13}^{13}(VW) = D_{13}^{13}(WV) ,$$

and,

$$D_{04}^{04}(V^2) = \left(D_{02}^{02}(V) \right)^2 .$$

Thus we have the configuration diagrams that will be used in this work.

V. RESULTS AND CONCLUSIONS

In this chapter we will discuss the results from the calculations of the first 6 radial moments of ^{16}O, ^{40}Ca, and ^{58}Ni.

A. Effect of the Model Space Size, Energy Dependence and ω Parameter

In this section we will study the effects of the model space size, energy dependence, and the starting energy ω parameter on the calculation of the expectation value of the radial moments $R^{(k)}(E)$.

Each of the single-particle harmonic oscillator orbitals that are in a given model space will be designated by the set of quantum numbers (n,ℓ,j), where n is the principal quantum number, ℓ is the orbital angular momentum quantum number, and $j = \ell \pm 1/2$ is the total angular momentum quantum number. When summing over orbitals, the degeneracy factor of $2j + 1$ is included to account for the z component of total angular momentum.

For the purpose of convenience in referring to the single-particle orbitals, we choose an order shown in Table 1 where the angular momentum quantum number ℓ is given in standard spectroscopic notation. A given model space is designated by the number p, and it contains all the single-particle orbitals up to and including these orbitals in the p-th shell, where $p = 2n + \ell$. (Whenever a model space contains in addition the first x orbitals of the next shell, then the model space will be referred to as p/x.)

Table 1. Single-particle orbitals used in model spaces

Number	n	ℓ	j	p = 2n + ℓ	N = Σ 2(2j+1)
1	0	S	1/2	0	4
2	0	P	1/2	1	8
3	0	P	3/2	1	16
4	1	S	1/2	2	20
5	0	D	3/2	2	28
6	0	D	5/2	2	40
7	1	P	1/2	3	44
8	1	P	3/2	3	52
9	0	F	5/2	3	64
10	0	F	7/2	3	80
11	2	S	1/2	4	84
12	1	D	3/2	4	92
13	1	D	5/2	4	104
14	0	G	7/2	4	120
15	0	G	9/2	4	140
16	2	P	1/2	5	144
17	2	P	3/2	5	152
18	1	F	5/2	5	164
19	1	F	7/2	5	180
20	0	H	9/2	5	200
21	0	H	11/2	5	224

The last column in Table 1 shows the running total of the number of unique orbitals N, where the isospin and total spin degeneracies are included.

If the radial moment operator $R^{(k)}$, which is defined in Eqs. (4.1) and (4.2), is divided by the number of particles m to give the normalization $\langle R^{(0)} \rangle \equiv 1$, then the moment $\langle R^{(k)} \rangle$ will be independent of the number of particles, with a dependence only on the number (N) and the type of orbitals (e.g., harmonic oscillator) N in the model space. Values for the moment $\langle R^{(2)} \rangle$ for an oscillator constant $\hbar\Omega$ = 14 MeV are given in Table 2.

Table 2. Values of the second moment of the radial operator as function of model space $\hbar\Omega$ = 14 MeV

Model Space	$\langle R^{(2)} \rangle (fm^2)$	$\langle R^{(2)} \rangle^{1/2} (fm)$
2	8.89	2.98
3	11.11	3.33
4	13.33	3.65
5	15.55	3.94

As will be seen, the moment $\langle R^{(k)} \rangle$ is usually the largest term in the truncated polynomial expansion for $R^{(k)}(E)$, Eq. (4.4), and since $\langle R^{(k)} \rangle$ increases with larger model spaces, the expectation value $R^{(k)}(E)$ increases also. We adopt the following prescription in order to further study the radial moments $R^{(k)}(E)$ for any given nucleus. We first choose the model space p/x so that $R^{(2)}(E)^{1/2}$ equals some desired root-mean-square radius and then study the behavior of $R^{(k)}(E)$ for $k \neq 2$. In

Table 3 we see the choices for Hamiltonians and model spaces which gave favorable root mean-square radii. Henceforward, we will use these Hamiltonians and model spaces for these nuclei. The calculated r_{rms} for ^{16}O, ^{40}Ca, and ^{58}Ni are compared with experimental charge radii (22) and also with mass radii from density dependent Hartree-Fock calculations (23).

With the expansion truncations discussed in Chapter IV, the energy dependence of the expectation values of the radial moments is linear, that is,

$$R^{(k)}(E) = A + B\,E \quad , \tag{5.1}$$

where

$$A = \langle R^{(k)} \rangle - \langle H \rangle (\langle R^{(k)} H \rangle - \langle R^{(k)} \rangle \langle H \rangle)/\sigma^2 \quad ,$$

$$B = (\langle R^{(k)} H \rangle - \langle R^{(k)} \rangle \langle H \rangle)\sigma^2 \quad ,$$

and $\sigma^2 = \langle H^2 \rangle - \langle H \rangle^2$, the width.

The energy E as an eigenvalue of the Hamiltonian is not known exactly. For the ground state energies, the experimental values (24) were used, where the Coulomb energy was removed by subtracting the semi-empirical mass formula (15) Coulomb energy term.

Tables 4, 5, and 6 list the values for the first 5 radial moments for the nuclei ^{16}O, ^{40}Ca, and ^{58}Ni, respectively, where the terms are defined in Eq. (5.1). The last column gives the percent change from the leading term $\langle R^{(k)} \rangle$ to the expectation value $R^{(k)}(E)$.

Table 3. Choices of model spaces and Hamiltonians

Nucleus	$R^{(2)}(E)^{1/2}$ (fm)	r_{rms}(DDHF) (fm)	r_{rms} (exp. charge) (fm)	Model Space	Hamiltonian Model Space	ω (MeV)
^{16}O	2.66	2.66	2.73	2	3	9
^{40}Ca	3.42	3.40	3.49	4/1	5	9
^{58}Ni	3.74	3.75	3.75	5	5	9

Table 4. Values for radial moments of ^{16}O, E = -142 MeV

Moment k	$\langle R^{(k)} \rangle (fm^k)$	$A(fm^k)$	$B(fm^k/MeV)$	$R^{(k)}(E)$ (fm^k)	% diff.
1	2.82	2.67	.129 E - 2	2.49	13
2	8.89	8.08	.711 E - 2	7.07	26
3	30.49	26.80	.323 E - 1	22.22	37
4	111.86	95.78	.141 E + 0	75.76	48
5	434.48	364.10	.617 E + 0	276.45	57

Table 5. Values for radial moments of ^{40}Ca, E = -416 MeV

Moment k	$\langle R^{(k)} \rangle (fm^k)$	$A(fm^k)$	$B(fm^k/MeV)$	$R^{(k)}(E)$ (fm^k)	% diff.
1	3.48	3.33	.195 E - 3	3.25	7
2	13.49	12.34	.154 E - 2	11.70	15
3	56.60	49.40	.905 E - 2	45.39	25
4	252.00	210.05	.562 E - 1	186.67	35
5	1177.65	938.72	.320 E + 0	805.55	46

Table 6. Values for radial moments of ^{58}Ni, E = -638 MeV

Moment k	$\langle R^{(k)} \rangle (fm^k)$	$A(fm^k)$	$B(fm^k/MeV)$	$R^{(k)}(E)$ (fm^k)	% diff.
1	3.74	3.61	.905 E - 4	3.55	5
2	15.55	14.47	.814 E - 3	13.95	11
3	69.57	62.31	.546 E - 2	58.83	18
4	329.01	283.74	.341 E - 1	262.01	26
5	1627.23	1352.22	.207 E + 0	1220.19	33

It should be noticed that with successive terms in Eq. (5.1), the expectation values of the radial moments decrease. It has been pointed out that this pattern has also been observed in moment calculations of spin cutoff factors (4,25).

For all three nuclei, the slope B of the linear relationship in the energy, Eq. (5.1), is seen to increase as the power k increases. Assuming an uncertainty of 1 MeV per nucleon we see in Tables 7, 8, and 9 the increase in the error in the radial moments with increasing k due to the uncertainty in the energy E. Because of this increase in error with increasing moments, we will choose to study the validity of only the first five moments.

Table 7. Error in radial moments of ^{16}O due to uncertainty of 1 MeV/nucleon in the ground state energy

Moment k	$R^{(k)}(E)(fm^k)$	$\Delta R^{(k)}(E)(fm^k)$	$\Delta R^{(k)}(E)/R^{(k)}(E)$ (%)
1	2.49	± .02	1
2	7.07	± .11	2
3	22.22	± .52	2
4	75.76	±2.26	3
5	276.45	±9.87	4

Finally, in Fig. 1 and Table 10 we see the dependence of the expectation value of the second radial moment $R^{(2)}(E)$ on the ω parameter in the Hamiltonian, where, for each of the three nuclei, the magnitude of the slope of the line between the extreme points is

$\tilde{\sim}$.01 fm^2/MeV. We conclude this dependence on ω is weak indeed and hence-forward will study results for ω = 9 MeV alone.

Table 8. Error in radial moments of ^{40}Ca due to uncertainty of 1 MeV/nucleon in ground state energy

Moment k	$R^{(k)}(E)(fm^k)$	$\Delta R^{(k)}(E)(fm^k)$	$\Delta R^{(k)}(E)/R^{(k)}(E)$ (%)
1	3.25	± .01	.2
2	11.70	± .06	1
3	45.39	± .39	1
4	186.67	± 2.25	1
5	805.55	±12.80	2

Table 9. Error in radial moments of ^{58}Ni due to uncertainty of 1 MeV/nucleon in the ground state energy

Moment k	$R^{(k)}(E)(fm^k)$	$\Delta R^{(k)}(E)(fm^k)$	$\Delta R^{(k)}(E)/R^{(k)}(E)$ (%)
1	3.55	± .01	.2
2	13.95	± .05	.3
3	58.83	± .32	1
4	262.01	± 1.98	1
5	1220.19	±12.01	1

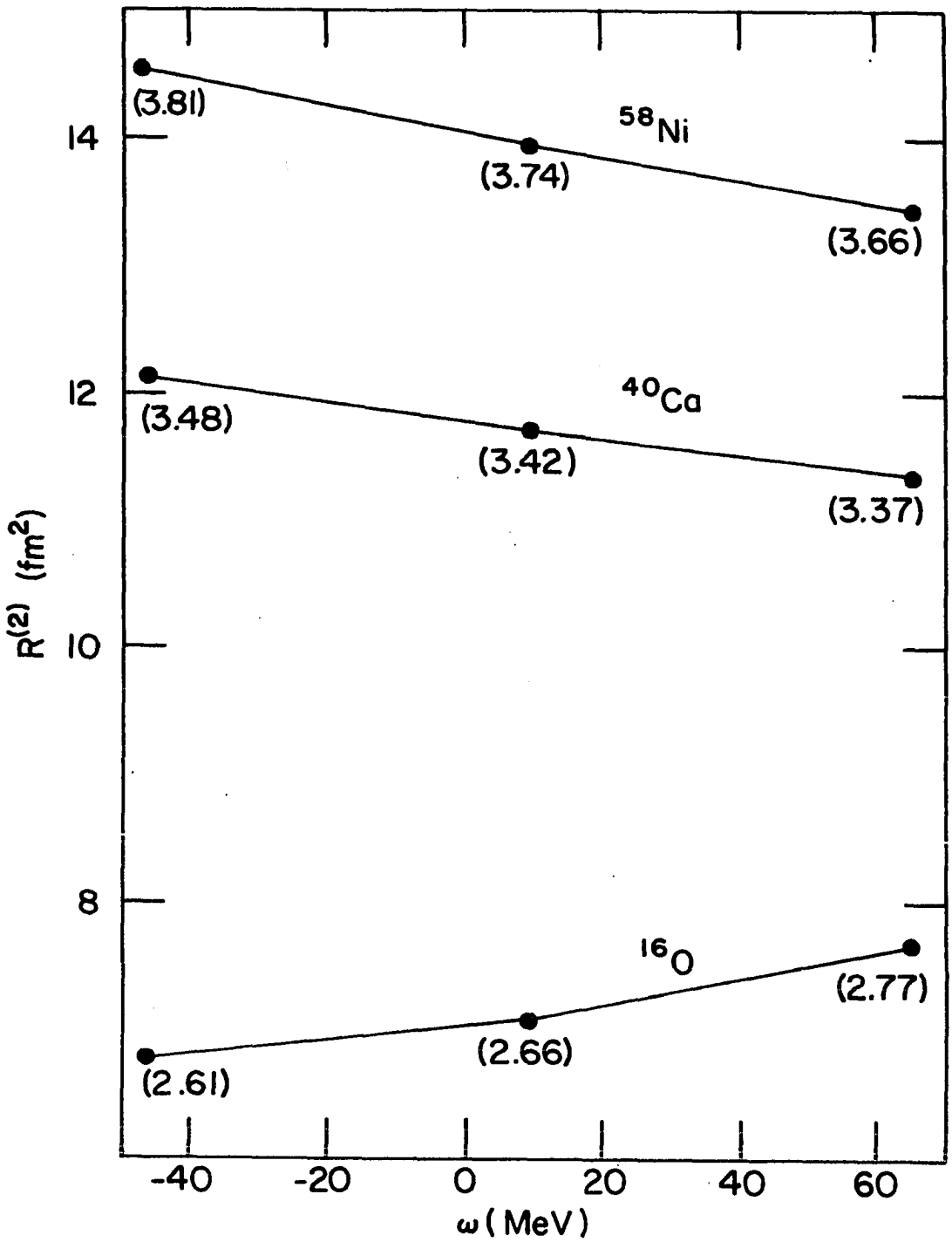

Figure 1. Dependence of the expectation value of the second radial moment on the starting energy ω

Table 10. Dependence of the second radial moment on the ω parameter

Nucleus	ω (MeV)	$R^{(2)}(E)$ (fm^2)	$(R^{(2)}(E)^{1/2}$ (fm)
^{16}O	-47	6.80	2.61
^{16}O	9	7.07	2.66
^{16}O	65	7.65	2.77
^{40}Ca	-47	12.13	3.48
^{40}Ca	9	11.70	3.42
^{40}Ca	65	11.37	3.37
^{58}Ni	-47	14.53	3.81
^{58}Ni	9	13.95	3.74
^{58}Ni	65	13.43	3.66

B. Comparisons with Other Calculations

In this section we compare expectation values of radial moments $R^{(k)}(E)$ with the radial moments

$$\langle r^k \rangle = \frac{4\pi}{m} \int_0^\infty \rho(r)\, r^{2+k}\, dr \quad ,$$

where $\rho(r)$ is the one-body mass density normalized so that $\langle r^0 \rangle \equiv 1$. The proton and neutron radial moments are given as

$$\langle r_p^k \rangle = \frac{4}{m_p} \int_0^\infty \rho_p(r)\, r^{2+k}\, dr$$

and

$$\langle r_n^k \rangle = \frac{4\pi}{m_n} \int_0^\infty \rho_n(r)\, r^{2+k}\, dr \quad ,$$

where $\rho_p(r)$ and $\rho_n(r)$ are the proton and neutron mass distributions, respectively, and are normalized so that $\langle r_p^0 \rangle = \langle r_n^0 \rangle \equiv 1$. Since the mass distribution is the sum of the proton and neutron distributions, we find that

$$\langle r^k \rangle = \frac{m_p}{m} \langle r_p^k \rangle + \frac{m_n}{m} \langle r_n^k \rangle \quad . \tag{5.2}$$

In Tables 11, 12, and 13 we see these comparisons with radial moments $\langle r^k \rangle$ of one-body densities of ^{16}O, ^{40}Ca, and ^{58}Ni, respectively from density dependent Hartree-Fock (23). We also compare with the results of 3 parameter Fermi distributions (22) whose parameters, given in Table 14, were chosen so that the first three radial moments are equal to the expectation value radial moments. In addition, in Tables 11 and 12 we include radial moments $\langle r^k \rangle$ of the one-body mass density $\rho(r)$ of the ground state, single Slater determinant wavefunction. We use spherical harmonic oscillator single-particle wavefunctions where the oscillator constant $\hbar\Omega$ was adjusted to give a second moment $\langle r^2 \rangle$ equal to $R^{(2)}(E)$.

In Fig. 2, for each of the three nuclei, we see a comparison of the 3 parameter Fermi densities and the DDHF densities.

C. Elastic Electron Scattering

In this section we apply a method used by Gordon (26) and input the expectation values of radial moments into an approximation of the elastic electron scattering form factor. We compare these results with experimental data (27,28,29) for ^{16}O, ^{40}Ca, and ^{58}Ni.

Table 11. Comparison of radial moments of ^{16}O

Moment k	$R^{(k)}(E)$	DDHF	3 Parameter Fermi	Ground State Slater Determinant $\hbar\Omega$ = 13.20 MeV
1	2.49	2.50	2.49	2.50
2	7.07	7.10	7.07	7.07
3	22.22	22.24	22.22	22.00
4	75.76	76.22	76.06	74.04
5	276.45	284.37	280.19	266.57

Table 12. Comparison of radial moments of ^{40}Ca

Moment k	$R^{(k)}(E)$	DDHF	3 Parameter Fermi	Ground State Slater Determinant $\hbar\Omega$ = 10.64 MeV
1	3.25	3.23	3.25	3.23
2	11.70	11.56	11.70	11.70
3	45.39	44.81	45.39	46.02
4	186.67	185.64	187.18	193.66
5	805.55	817.79	813.40	862.85

Table 13. Comparison of radial moments of ^{58}Ni

Moment k	$R^{(k)}(E)$	DDHF	3 Parameter Fermi
1	3.55	3.58	3.55
2	13.95	14.05	13.94
3	58.83	59.23	58.83
4	262.01	265.01	262.49
5	1220.19	1251.00	1224.76

Table 14. Parameters of the 3 parameter Fermi distribution $\rho(r) = \rho_0(1 + wr^2/c^2)(1 + \exp[(r - c)/z])^{-1}$

Nucleus	$\rho_0(fm^{-3})$	c(fm)	z(fm)	w
^{16}O	.176	2.626	.514	-.113
^{40}Ca	.160	4.033	.480	-.254
^{58}Ni	.181	4.516	.541	-.343

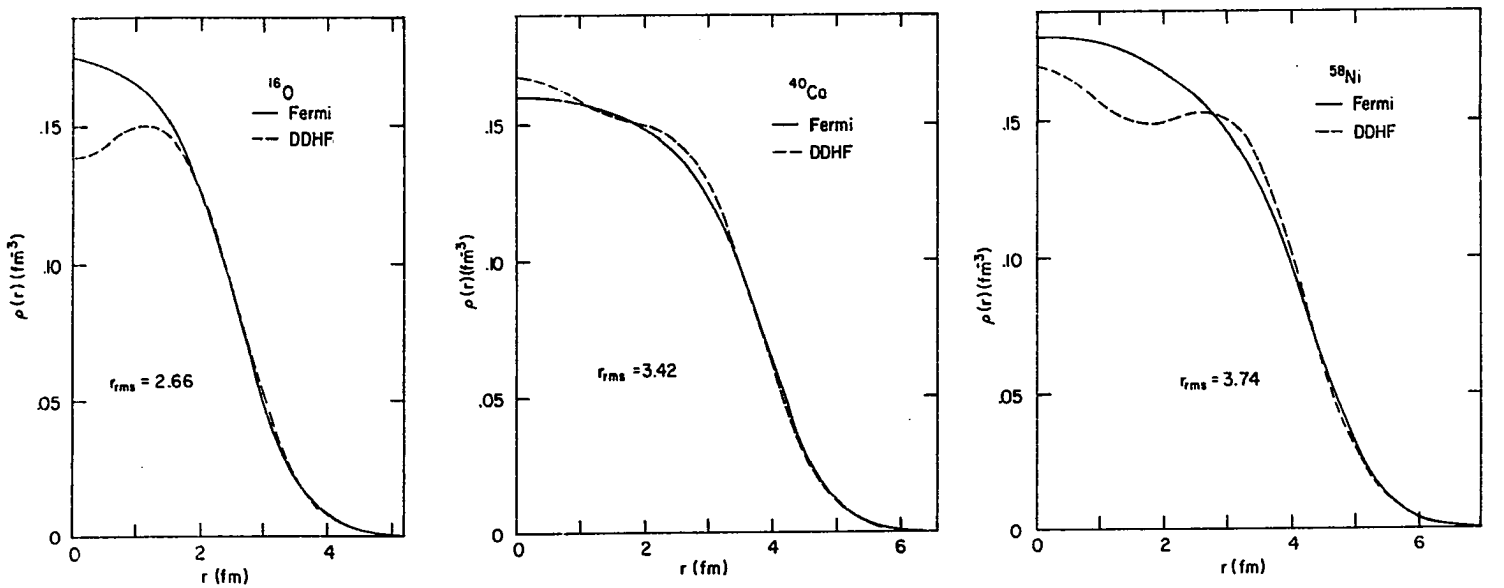

Figure 2. Comparison of DDHF density distributions with 3 parameter Fermi distributions

The elastic electron scattering form factor, in the first Born approximation (22), is given by

$$F(q) = \frac{4\pi}{m_p} \int_0^\infty \rho_c(r) \frac{\sin qr}{qr} r^2 \, dr \quad , \tag{5.3}$$

where $\rho_c(r)$ is the change distribution of the nucleus normalized so that

$$\frac{4\pi}{m_p} \int_0^\infty \rho_c(r) \, r^2 \, dr \equiv 1 \quad .$$

Also, q is the amplitude of the four-momentum transfer.

The differential cross section is given by

$$\frac{d\sigma}{d\Omega} = \frac{d\sigma}{d\Omega_{Mott}} |F(q)|^2 \quad ,$$

where $d\sigma/d\Omega_{Mott}$ is the differential elastic scattering cross section from a point nucleus with no spin.

This application of the technique of Gordon's employs the conventionally defined set of radial charge moments

$$\langle r_c^k \rangle = \frac{4\pi}{m_p} \int_0^\infty \rho_c(r) \, r^{2+k} \, dr \quad , \quad k = 0, \ldots, C \tag{5.4}$$

to determine the set $\{\rho_i, \zeta_i\}_{i=1}^d$ of weights and mesh points of a weighted delta distribution

$$\bar{\rho}(r) = \sum_{i=1}^{d} \rho_i \, \delta(r - \zeta_i) \quad .$$

The set is chosen so that the first C + 1 radial moments of the weighted delta distribution equal the radial charge moments of $\rho(r)$. The

integral in Eq. (5.3) is then approximated by

$$F(q)^{(C)} = \frac{4\pi}{m_p} \sum_{i=1}^{d} \rho_i \frac{\sin(q\zeta_i)}{q\zeta_i} \quad . \tag{5.5}$$

Before we adopt the Gordon method to our problem, we demonstrate its convergence properties as a function of the number of radial moments C. This demonstration is facilitated by choosing a Gaussian charge density

$$\rho(r) = \rho_0 \exp(- P^2 r^2) \quad ,$$

whose form factor can be written analytically (30) as

$$F(q) = \exp(- q^2/4P^2) \quad . \tag{5.6}$$

The parameters ρ_0 and P^2 were chosen so that

$$\int_0^\infty \rho(r)\, r^2\, dr = 1$$

and

$$\int_0^\infty \rho(r)\, r^4\, dr = r_{rms}^2 \quad .$$

In order to make the convergence test realistic we choose the root-mean-square charge radius r_{rms} of either ^{16}O or ^{40}Ca and use q values which are the same as for the experimental data which we have selected to study below.

To summarize the convergence demonstration we proceed as follows; select a Gaussian one-body density $\rho(r)$, fix its parameters to the

experimental r_{rms}, evaluate Eq. (5.4) for k = 1, ..., C, obtain the set $\{\rho_i, \zeta_i\}$ according to the method of Gordon, and then evaluate Eq. (5.5) and compare the results as a function of C with the analytic result Eq. (5.6).

The results in Tables 15 and 16 demonstrate that, for the lowest q value, the form factor $F(q)^{(5)}$ has converged to roughly 3 and 4 significant digits for ^{16}O and ^{40}Ca, respectively. For the lower q values, in general, the results converged better, for a fixed number of radial charge moments.

Table 15. Convergence of form factor for lowest scattering angle, using a Gaussian density distribution, $E_{electron}$ = 2493 MeV, $r^{(2)}_{rms}$ = 11.70 fm^2

Angle (degrees)	q Value (fm^{-1})	F(q) Analytic	$F(q)^{(3)}$	$F(q)^{(5)}$	$F(q)^{(7)}$
24.08	.527	.58194	.58203	.58191	.58194

Table 16. Convergence of form factor for lowest scattering angle, using a Gaussian density distribution, $E_{electron}$ = 374 MeV, $r^{(2)}_{rms}$ = 7.07 fm^2

Angle (degrees)	q Value (fm^{-1})	F(q) Analytic	$F(q)^{(3)}$	$F(q)^{(5)}$	$F(q)^{(7)}$
32	1.04	.27668	.28907	.27554	.27674

With this in mind we now proceed to describe the results obtained when the expectation values of radial moments $R^{(k)}(E)$, given

in Eq. (5.1), are employed as input quantities for $\langle r_c^k \rangle$. In this case we do not know the one-body density distribution function but only its lower radial moments.

By proceeding in this fashion, we are assuming the proton to be a point charge so that $\langle r_c^k \rangle = \langle r_p^k \rangle$. We will correct for this assumption later. Further, for ^{16}O and ^{40}Ca, we see by Eq. (5.2) that the proton density equals the neutron density with the Coulomb free Hamiltonian so that the radial moments of the mass distribution are the same as the charge radial moments. For ^{58}Ni we employ the commonly made assumption that $\rho_p(r) = m_p/m_n \, \rho_n(r)$.

The differential elastic electron scattering cross section has been determined with the Gordon method, using C = 5, for ^{16}O, ^{40}Ca, and ^{58}Ni, and the results are displayed with experimental data in Fig. 3. The overall agreement between theory and experiment must be reviewed in light of our approximations.

For example, assuming the proton form factor to be of the form (15)

$$G_E(q) = (1 + aq^2)^{-2} \quad , \tag{5.7}$$

where a = .055 fm^2, the theoretical cross sections shown in Fig. 3 can be corrected for the finite proton charge distribution by multiplying by Eq. (5.7). Tables 17, 18, and 19 compare the experimental results for smaller scattering angles with those corrected results. It is observed that this correction improves agreement between theory and experiment in the region of low q-values where the truncation at C = 5 is most acceptable.

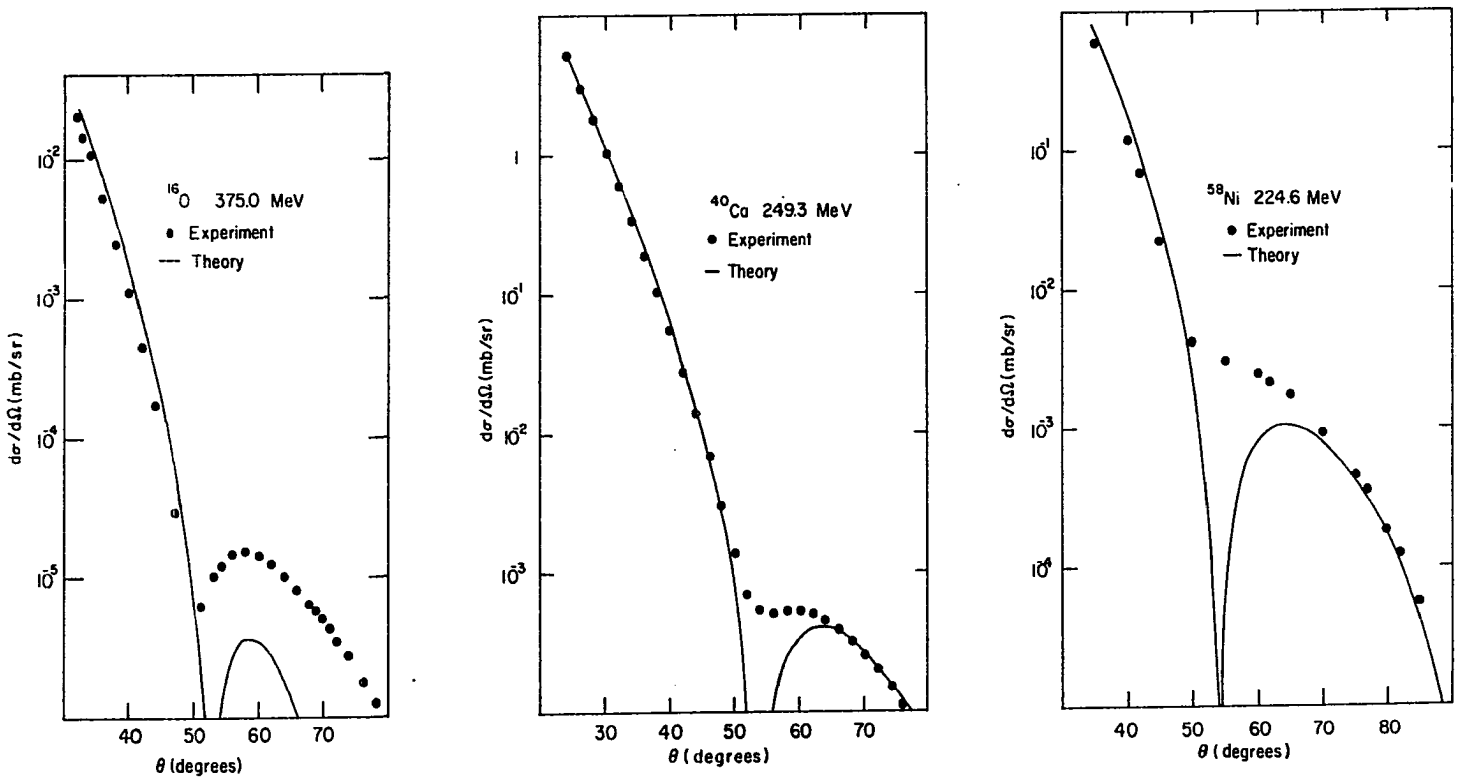

Figure 3. Elastic electron scattering cross sections, comparison of theory with experimental data

Table 17. Elastic electron scattering cross section on ^{16}O, $E_{electron}$ = 374.5 MeV

Lab Scattering Angle (degrees)	q Value (fm^{-1})	$d\sigma/d\Omega_{exp}$ (mb/sr)	$error_{exp}$ (mb/sr)	$d\sigma/d\Omega_{thy}$ (mb/sr)
32	1.044	.198 E - 1	.400 E - 3	.210 E - 1
34	1.107	.103 E - 1	.200 E - 3	.110 E - 1
36	1.170	.521 E - 1	.110 E - 3	.561 E - 2

Table 18. Elastic electron scattering cross section on ^{40}Ca, $E_{electron}$ = 249.3 MeV

Lab Scattering Angle (degrees)	q Value (fm^{-1})	$d\sigma/d\Omega_{exp}$ (mb/sr)	$error_{exp}$ (mb/sr)	$d\sigma/d\Omega_{thy}$ (mb/sr)
24.08	.527	.527 E + 1	.15 E + 0	.521 E + 1
28.08	.613	.181 E + 1	.61 E - 1	.179 E + 1
32.08	.698	.614 E + 0	.20 E - 1	.605 E + 0

Table 19. Elastic electron scattering cross section on ^{58}Ni, $E_{electron}$ = 224.6 MeV

Lab Scattering Angle (degrees)	q Value (fm^{-1})	$d\sigma/d\Omega_{exp}$ (mb/sr)	$error_{exp}$ (mb/sr)	$d\sigma/d\Omega_{thy}$ (mb/sr)
35	.685	6.11 E - 1	.42 E - 1	6.95 E - 1
40	.780	1.25 E - 1	.09 E - 1	1.56 E - 1
42	.817	6.87 E - 2	.47 E - 2	8.05 E - 2

The impact of correcting for the other approximations (Born approximation and polynomial series truncation) may not be so favorable. This will be discussed along with our conclusions.

D. Conclusion

We have used the moments of operators in the truncated orthogonal polynomial expansion, given in Eq. (5.1), to calculate the expectation values of the first 6 radial moments. We have applied the method to effective nuclear Hamiltonians for the nuclei ^{16}O, ^{40}Ca, and ^{58}Ni and have obtained results which are reasonable in two ways. First, as shown in Section B, these 6 moments agree with those of phenomenologically successful one-body density distributions. Second, as shown in Section C, those radial moments yield satisfactory predictions of the elastic electron scattering cross sections of those nuclei.

One major limiting feature of our application has emerged. Recalling the results of Table 2, we demonstrated sensitivity of the second radial moment $\langle R^{(2)} \rangle$ to the model space size. This is true of the other radial moments $\langle R^{(k)} \rangle$ as well. These quantities are independent of the number of nucleons so if we had a fixed model space for all nuclei we would be initiating an expansion for the radial moment expectation value about the same value, independent of nucleus. Obviously, different convergence rates would be expected if this procedure were followed. So, instead of a fixed model space for all nuclei, we adopt a perscription choosing the model space size which gives a desired root-mean-square radius for the particular nucleus. The eigenenergies of the ground states for our effective Hamiltonians are not known

exactly. Hence we used the Coulomb corrected experimental binding energies in the truncated expansion in Eq. (5.1). This should be satisfactory since we found the lowest radial moments have only a weak dependence on changes in the ground state energy.

We have tested the method of Gordon and found it applicable to developing the elastic electron scattering cross section directly from expectation values of radial moments. With the Gordon method, using the first 6 radial moment expectation values, we saw that the calculated cross sections for the lowest q values was within error bounds for the experimental cross section of the ^{40}Ca case, and about 5 % larger than the experimental cross section for both the ^{16}O and the ^{58} Ni cases.

The first Born approximation is valid for $z/137 << 1$ and its application to scattering on ^{58}Ni is probably subject to 10% corrections. The model space size for the ^{16}O calculation was considerably smaller than for ^{40}Ca and ^{58}Ni and this could explain the greater discrepancy between theory and data.

Independence of model space size is a desired goal of a theory with true predictive power. Clearly, this goal can be achieved only by including additional terms in the orthogonal polynomial expansion in Eq. (4.7). Including just the next term will require the calculation of the higher Hamiltonian moments $\langle H^3 \rangle$ and $\langle H^4 \rangle$. This is not feasible at the present time (31).

Once convergence of the orthogonal polynomial expansion, as well as independence from model space size, is achieved, it would be appropriate to extend these methods to other operators of physical

interest. General multipole moments of the one-body density and moments of the two-body density (correlation information) immediately spring to mind. We have seen here the tantalizing prospects of what a continued effort in this direction may yield.

VI. APPENDIX A: WICK'S THEOREM

Wick's theorem (21) presents a systematic method for evaluating m-particle matrix elements which involve products of creation and destruction operators.

The statement of the theorem involves two definitions. The first one, called the normal ordered product of operators, is a product derived from any given product of creation and destruction operators by moving the creation operators to the left of the destruction operators and then including a factor of +(-)1 if an even (odd) number of permutations of operators is involved. As an example, the normal ordering of the product $a_\alpha b_\beta a_\gamma b_\delta$ is

$$N(a_\alpha b_\beta a_\gamma b_\delta) = (-1)^P a_\alpha a_\gamma b_\beta b_\delta \quad , \tag{A.1}$$

where the number of permutations P required to give the normal ordering is 1.

The second definition used in Wick's theorem concerns the contraction of two given operators which are in a product of operators, and this is simply the matrix element of the two operators with respect to the vacuum $|0\rangle$, times a factor of +(-)1 depending upon whether an even or odd number of permutations P is required to bring the two operators together in the product. For an example, we will contract the operators b_β and a_γ in the product $a_\alpha b_\beta a_\gamma b_\delta$, that is

$$\begin{aligned} a_\alpha \overbrace{b_\beta a_\gamma} b_\delta &= (-1)^P a_\alpha \langle 0|b_\beta a_\gamma|0\rangle b_\delta \\ &= (-1)^0 \delta_{\beta\gamma} a_\alpha b_\delta \quad . \end{aligned} \tag{A.2a}$$

If more than one contraction of pairs of operators is taken within a product, the contractions may be taken in any order, and the previously contracted pairs won't contribute to any subsequent contractions. For example, we can contract the operators a_α and b_δ in Eq. (A.2) so that

$$\begin{aligned} \overbrace{a_\alpha b_\beta a_\gamma b_\delta} &= (-1)^P \overbrace{a_\alpha b_\delta} b_\beta a_\gamma \\ &= (-1)^2 \langle 0|a_\alpha b_\delta|0\rangle\langle 0|b_\beta a_\gamma|0\rangle \quad . \end{aligned} \tag{A.2b}$$

If one or more contractions are taken within a normal ordered product, the contractions, as described in the preceeding two paragraphs, will be made first, and followed by the normal ordering of the uncontracted operators in the product. For example, if we contract the operators b_β and a_γ in Eq. (A.1), we see that

$$\begin{aligned} N(a_\alpha \overbrace{b_\beta a_\gamma} b_\delta) &= (-1)^P \overbrace{b_\beta a_\gamma} N(a_\alpha b_\gamma) \\ &= (-1)^0 \delta_{\beta\gamma} a_\alpha b_\gamma \quad . \end{aligned} \tag{A.3}$$

Now, Wick's theorem states that the product of any number of creation and destruction operators is equal to the sum of all possible contractions of the normal ordered product, including full, partial, and no contractions.

One of the simplest examples of the application of Wick's theorem involves the matrix element of $a_\alpha b_\beta$ with respect to the vacuum $|0\rangle$, that is

$$\begin{aligned}\langle 0|b_\alpha a_\beta|0\rangle &= \langle 0|N(b_\alpha a_\beta) + N(\overbrace{b_\alpha b_\beta})|0\rangle \\ &= \langle 0|a_\alpha b_\beta + \langle 0|b_\alpha a_\beta|0\rangle N(0)|0\rangle \\ &= \langle 0|b_\alpha a_\beta|0\rangle \quad . \end{aligned} \tag{A.4}$$

For the matrix element of a product of two creation and two destruction operators, we see that

$$\begin{aligned}\langle 0|b_\alpha a_\beta b_\gamma a_\delta|0\rangle = \langle 0|(&N(b_\alpha a_\beta b_\gamma a_\delta) + N(\overbrace{b_\alpha a_\beta} b_\gamma a_\delta) + N(\overbrace{b_\alpha a_\beta b_\gamma a_\delta}) \\ &+ N(b_\alpha a_\beta \overbrace{b_\gamma a_\delta}) + N(b_\alpha \overbrace{a_\beta b_\gamma} a_\delta) + N(\overbrace{b_\alpha a_\beta} \overbrace{b_\gamma a_\delta}) \\ &+ N(\overbrace{b_\alpha a_\beta b_\gamma a_\delta})|0\rangle \quad , \end{aligned}$$

where the terms with contractions between like operators are not included because they yield zero.

The definitions of normal ordering and contracted pairs may be applied to write

$$\begin{aligned}\langle 0|b_\alpha a_\beta b_\gamma a_\delta|0\rangle &= \langle (0|(-1)^3 a_\beta a_\delta b_\alpha b_\gamma + (-1)^2 \overbrace{b_\alpha a_\beta}(-1)^1 a_\delta b_\gamma \\ &\quad + (-1)^2 \overbrace{b_\alpha a_\delta}(-1)^0 a_\beta b_\gamma + (-1)^0 \overbrace{b_\gamma a_\delta}(-1)^1 a_\beta b_\alpha \\ &\quad + (-1)^0 a_\beta b_\gamma (-1)^1 a_\delta b_\alpha + (-1)^0 \overbrace{b_\alpha a_\beta}(-1)^0 \overbrace{b_\gamma a_\delta} \\ &\quad + (-1)^2 \overbrace{b_\alpha a_\delta} \overbrace{a_\beta b_\gamma}|0\rangle \\ &= \delta_{\alpha\delta}\delta_{\beta\gamma} \quad , \end{aligned} \tag{A.5}$$

where only the next to last term was nonzero.

Note that because normal ordering places the destruction operators to the right of the product and since $b_\alpha|0\rangle = 0$ for any state labeled α, when applying Wick's theorem to matrix elements with the vacuum $|0\rangle$,

only the fully contracted terms may possibly be nonzero, and all other terms with partial or no contractions may be dropped.

VII. APPENDIX B: RELATIVE KINETIC ENERGY OPERATOR

First we write the total kinetic energy as

$$0 = \sum_{i=1}^{m} \frac{p_i^2}{2m} \tag{B.1}$$

where p_i^2 is the square of the momentum of the i-th particle and m is the nucleon mass. We can also define the total kinetic energy as the sum of the kinetic energy due to the center of mass motion and kinetic energy due to the motion of the particle relative to the center of mass,

$$0 = T_{CM} + T_{Rel} \quad . \tag{B.2}$$

Since the center of mass momentum is

$$\vec{P}_{CM} = \sum_{i=1}^{m} \vec{p}_i \quad ,$$

we can write

$$T_{CM} = \frac{P_{CM}^2}{2M} = \sum_{i,j=1}^{m} \frac{\vec{p}_i \cdot \vec{p}_j}{2M} \quad , \tag{B.3}$$

where M = m x m is the total mass.

This allows Eq. (B.2) to be written as

$$T_{Rel} = \sum_{i=1}^{m} \frac{p_i^2}{2M} - \frac{1}{m} \sum_{i,j=1}^{m} \frac{\vec{p}_i \cdot \vec{p}_j}{2M} \quad . \tag{B.4}$$

Rewriting the first term in Eq. (B.4) as

$$\sum_{i=1}^{m} \frac{p_i^2}{2M} = \frac{1}{2M} \sum_{i,j=1}^{m} \left(\frac{p_i^2}{2M} + \frac{p_j^2}{2M} \right)$$

gives

$$T_{Rel} = \frac{1}{8m\mu} \sum_{i,j=1}^{m} (p_i^2 + p_j^2 - 2\underline{p}_i \cdot \underline{p}_j) \quad , \tag{B.5}$$

where $\mu = M/2$ is the reduced mass.

Defining the relative momentum between the i-th and j-th particles as

$$\vec{p}_{ij} = \frac{1}{2} (\vec{p}_i - \vec{p}_j)$$

allows Eq. (B.5) to be written as

$$T_{Rel} = \frac{1}{m} \sum_{i,j=1}^{m} \frac{p_{ij}^2}{2\mu} \quad . \tag{B.6}$$

VIII. APPENDIX C: TRACE FORMULAS

In this appendix we will develop trace formulas for both the scalar and configuration m-body traces of a general k-body operator O(k).

A general k-body operator O(k) will be defined in the operator representation as

$$O(k) = \sum_{\substack{\alpha,\ldots,\delta \\ \mu,\ldots,\omega}} O^{\omega,\ldots,\mu}_{\alpha,\ldots,\delta}\, a_\alpha \ldots a_\delta b_\mu \ldots b_\omega \quad , \tag{C.1}$$

where there are k creation operators as well as k destruction operators, and the coefficients $O^{\omega,\ldots,\mu}_{\alpha,\ldots,\delta}$ are <u>not necessarily</u> antisymmetric under the exchange of any two superscripts or any two subscripts.

By placing Eq. (C.1) into Eq. (3.13), we see that the scalar trace of O(k) can be written as

$$\langle\langle O(k)\rangle\rangle_{S(m)} = \sum_{\Gamma=1}^{d_m} \sum_{\substack{\alpha,\ldots,\delta \\ \mu,\ldots,\omega}} O^{\omega,\ldots,\mu}_{\alpha,\ldots,\delta} \langle\Gamma| a_\alpha \ldots a_\delta b_\mu \ldots b_\omega |\Gamma\rangle \quad . \tag{C.2}$$

We will denote the single particle state labels of the m-particle state with lower case Roman letters so that upon applying Wick's theorem (Appendix A) to the diagonal matrix element with the state Γ in Eq. (C.2), we can write the matrix element as

$$\langle\Gamma| a_\alpha \ldots a_\delta b_\mu \ldots b_\omega |\Gamma\rangle = \sum_{(i,\ldots,j)\in S(\Gamma)} \langle 0| b_1 \ldots \overline{b_i} \ldots \overline{b_j} \ldots b_m (\overline{a_\alpha} \ldots \overline{a_\delta} \overline{b_\mu} \ldots \overline{b_\omega}) a_m \ldots \overline{a_j} \ldots \overline{a_i} \ldots a_1 |0\rangle \quad , \tag{C.3}$$

where $(i,\ldots,j)\in S(\Gamma)$ is the set of all k single-particle labels that

are in the set of m single-particle labels in the state Γ. The broken contractions in Eq. (C.3) denote all possible contractions between the k creation (destruction) operators with labels $\alpha,\ldots,\delta$ ($\mu,\ldots,\omega$) and the k destruction (creation) operators with labels $i,\ldots,j$ ($i,\ldots,j$). The creation operators with the remaining (m-k) labels that belong to the state Γ can only contract with destruction operators with like labels, e.g., $b_1 a_1 = \langle 0|b_1 a_1|0\rangle = 1$, and upon making these (m-k) contractions, where each one yields unity, so these operators may simply be removed from the matrix element in Eq. (C.3), we can then write the trace, which is Eq. (C.2), as

$$\langle\langle O(k)\rangle\rangle_{S(m)} = \sum_{\Gamma=1}^{d_m} \sum_{(i,\ldots,j)\in S(\Gamma)} \sum_{\substack{\alpha,\ldots,\delta \\ \mu,\ldots,\omega}} O^{\omega,\ldots,\mu}_{\alpha,\ldots,\delta} \times \langle i,\ldots,j|a_\alpha \ldots a_\delta b_\mu \ldots b_\omega|i,\ldots,j\rangle \quad . \tag{C.4}$$

Each set of k labels $(i,\ldots,j)$ can be associated with a k-particle state vector $|i,\ldots,j\rangle$, and in the sum over $(i,\ldots,j)\in S(\Gamma)$ there will be a total of $\binom{m}{k}$ unique k-particle state vectors. The double sum over state $\Gamma\in S(m)$ and all sets of k labels $(i,\ldots,j)\in S(\Gamma)$, in Eq. (C.4) will involve all N single particle orbitals and will contain every k-particle state that belongs to the space

$$S(k) = \{|\Lambda\rangle; \Lambda = 1, \ldots, d_k\} \quad . \tag{C.5}$$

The k-particle state in S(k) are constructed by filling N orbitals with k identical particles in all possible ways. The dimensionality of S(k)

will then be $d_k = \binom{N}{k}$. In that double sum in Eq. (D.4) <u>each</u> k-particle state will appear R times since a given set of R m-particle states will each contain the same ordered set of k labels. Since there are $\binom{N}{m}$ m-particle states in S(m) and $\binom{m}{k}$ k-particle states in each m-particle state, there will appear $\binom{N}{m}\binom{m}{k}$ k-particle states in the double sum. With $\binom{N}{k}$ unique k-particle states in S(k), we find the multiple occurrence R of each k-particle state to be

$$R = \frac{\binom{N}{m}\binom{m}{k}}{\binom{N}{R}} = \binom{N-k}{m-k} \quad . \tag{C.6}$$

That double sum in Eq. (C.4) can then be replaced by a single sum over all k-particle states in S(k) times R, so that Eq. (C.4) becomes

$$\langle\langle O(k)\rangle\rangle_{S(m)} = \binom{N-k}{m-k}\langle\langle O(k)\rangle\rangle_{S(k)} \quad , \tag{C.7a}$$

where we have defined the k-particle trace as

$$\langle\langle O(k)\rangle\rangle_{S(k)} = \sum_{\Lambda\epsilon S(k)} \sum_{\substack{\alpha,\ldots,\delta \\ \mu,\ldots,\omega}} O^{\mu,\ldots,\omega}_{\alpha,\ldots,\delta} \langle\Lambda|a_\alpha\ldots a_\delta b_\mu\ldots b_\omega|\Lambda\rangle \quad . \tag{C.7b}$$

We can apply Wick's theorem, further, to the k-particle diagonal matrix element in Eq. (C.7b) to reduce it to the following contractions.

$$\langle 0|b_i\ldots b_j(a_\alpha\ldots a_\delta b_\mu\ldots b_\omega)a_j\ldots a_i|0\rangle = PP'(-1)^P(01)^{P'}\Delta^{\omega,\ldots,\mu}_{j,\ldots,i\ \alpha,\ldots,\delta} \quad . \tag{C.7c}$$

where P(P') is the permutation operator which creates k!(k!) terms with all possible permutations of the superscript (subscript) labels, and

p(p') is the number of permutations of the respective labels for a given term. The function $\Delta^{\omega,\ldots,\mu}_{\alpha,\ldots,\delta}{}_{j,\ldots,i}$ is unity if the three labels in each column are equal, and is zero otherwise. Placing these contractions into Eq. (C.7b) and taking the sum over the labels $\alpha,\ldots,\delta$, and $\mu,\ldots,\omega$, we can write the k-particle trace as

$$\ll O(k) \gg_{S(k)} = \sum_{(i,\ldots,j)\varepsilon S(k)} PP'(-1)^{P}(-1)^{P'} O^{k,\ldots,i}_{k,\ldots,i} \quad . \text{(C.7d)}$$

If the coefficients $O^{\omega,\ldots,\delta}_{\alpha,\ldots,\delta}$ are antisymmetric under the exchange of adjacent superscripts and also the exchange of adjacent subscripts, then <u>each</u> of the $k!^2$ terms that are generated by the permutation operators P and P' in Eq. (C.7d) will be equal to $O^{i,\ldots,k}_{i,\ldots,k}$. So, we can write the k-particle scalar trace as

$$\ll O(k) \gg_{S(k)} = (k!)^2 \sum_{(i,\ldots,j)\varepsilon S(k)} O^{i,\ldots,j}_{i,\ldots,j} \quad . \qquad \text{(C.8a)}$$

Further, since the coefficient $O^{i,\ldots,k}_{i,\ldots,k}$, which is in Eq. (C.8a) is <u>symmetric</u> under the permutation of any two columns of labels, yet the coefficient is zero if any two columns are equal, in the previous equation, we can unrestrict the sum over single-particle orbitals, which are in Eq. (C.8a), if we divide by k!, which is the number of redundant terms. Thus, for antisymmetric coefficients, we can write the k-particle trace as

$$\ll O(k) \gg_{S(k)} = k! \sum_{i,\ldots,j} O^{i,\ldots,j}_{i,\ldots,j} \quad , \qquad \text{(C.8b)}$$

where the unrestricted sum over the k labels i,...,j includes all N single-particle orbitals.

For a one-body operator O(1), which is defined in Eqs. (2.32) and (2.34), we can apply Eqs. (C.7) and (C.8) and write the scalar trace as

$$\langle\langle O(1)\rangle\rangle_{S(m)} = \binom{N-1}{m-1} \sum_{\alpha} O_{\alpha\alpha} \quad . \tag{C.9}$$

For a two-body operator O(2), which is defined in Eqs. (2.35) and (2.37), we can again apply Eqs. (C.7) and (C.8) and write the scalar trace as

$$\langle\langle O(2)\rangle\rangle_{S(m)} = \binom{N-2}{m-2} 2 \sum_{\alpha\beta} O_{\alpha\beta\beta\alpha} \quad . \tag{C.10}$$

For obtaining the configuration trace of the k-body operator O(k), we begin by placing Eq. (C.1) into Eq. (3.34). We then can write

$$\langle\langle O(k)\rangle\rangle_{S(\vec{m})} = \sum_{\Gamma\epsilon S(\vec{m})} \sum_{\substack{\alpha,\ldots,\delta \\ \mu,\ldots,\omega}} O^{\omega,\ldots,\mu}_{\alpha,\ldots,\delta} \langle\Gamma|a_\alpha \ldots a_\delta b_\mu \ldots b_\omega|\Gamma\rangle \quad . \tag{C.11}$$

We will let the single-particle labels of the m-particle state Γ be denoted by lower case Roman letters and then use Wick's theorem to write the diagonal matrix element in Eq. (C.11) as

$$\langle\Gamma|a_\alpha \ldots a_\delta b_\mu \ldots b_\omega|\Gamma\rangle =$$

$$\sum_{(\vec{k})} \sum_{(i,\ldots,j)_{\vec{k}}\epsilon S(\Gamma)} \langle 0|b_1 \ldots \overline{b_i} \ldots \overline{b_j} \ldots b_m (\overline{a_\alpha} \ldots \overline{a_\delta} \overline{b_\mu} \ldots \overline{b_\omega}) a_m \ldots \overline{a_j} \ldots \overline{a_i}$$

$$\times \ldots a_1|0\rangle \quad . \tag{C.12}$$

In this equation we have defined $(\vec{k})$ as the set of all configurations $k = (k_1, k_2, \ldots, k_\ell)$, where $k_1 \leq m_1, \ldots, k_\ell \leq m_\ell$ and $k_1 + k_2 + \ldots + k_\ell = k$.

In Eq. (C.12), we use $(i,\ldots,j)_{\vec{k}}\varepsilon(\Gamma)$ to indicate the set of all k single-particle labels that belong to the set of m single particle labels in the state Γ and also to the configuration $\vec{k}$. The broken contractions in Eq. (C.12) denote all possible contractions between the k creation (destruction) operators with labels $\alpha,\ldots,\delta$ $(\mu,\ldots,\omega)$ and the k destruction (creation) operators with labels $i,\ldots,j$ $(i,\ldots,j)$. Upon making the contractions between the (m-k) creation and destruction operators with the same labels, these contracted operators can be removed from Eq. (C.12) so that the trace in Eq. (C.11) becomes

$$\langle\langle O(k)\rangle\rangle_{S'(m)} = \sum_{(\vec{k})} \sum_{\Gamma\varepsilon S'(\vec{m})} \sum_{(i,\ldots,j)_{\vec{k}}\varepsilon S(\Gamma)} \sum_{\substack{\alpha,\ldots,\delta \\ \mu,\ldots,\omega}} O^{\omega,\ldots,\mu}_{\alpha,\ldots,\delta} \times \langle i,\ldots,j|a_\alpha\ldots a_\delta b_\mu\ldots b_\omega|i,\ldots,j\rangle \quad . \tag{C.13}$$

Now, each set of labels $(i,\ldots,j)_{\vec{k}}$ can be associated with a k-particle state vector $|i,\ldots,j\rangle$, and in the sum over $(i,\ldots,j)_{\vec{k}}\varepsilon S(\Gamma)$ there will be a total of

$$\left[\binom{m_1}{k_1}\ldots\binom{m_\ell}{k_\ell}\right]_{\vec{k}}$$

unique k-particle state vectors. The double sum over states $\Gamma\varepsilon S(\vec{m})$ and all sets of labels $(i,\ldots,j)_{\vec{k}}\varepsilon S(\Gamma)$, in Eq. (C.13) will involve all N single-particle orbitals and will contain every k-particle state that belongs to the k-particle configuration space

$$S(\vec{k}) = \{|\Lambda\rangle,\ \Lambda = 1,\ \ldots,\ d_{\vec{k}}\} \quad . \tag{C.14}$$

The k-particle states in $S(\vec{k})$ are constructed by filling N_1 orbitals with k_1 identical particles in all possible ways, and likewise for the other ℓ-1 partitions. The dimensionality of $S(\vec{k})$ will then be

$$d_{\vec{k}} = \left[\binom{N_1}{k_1} \binom{N_2}{k_2} \cdots \binom{N_\ell}{k_\ell} \right]_{\vec{k}} \quad . \tag{C.15}$$

In that double sum in Eq. (C.13), <u>each</u> k-particle state that belongs to $S(\vec{k})$ will appear $R_{\vec{k}}$ times, since a given set of $R_{\vec{k}}$ m-particle states that belong to $S(\vec{m})$ will each contain the same ordered set of k labels. Since there are $[\binom{N_1}{m_1} \cdots \binom{N_\ell}{m_\ell}]$ m-particle states in $S(\vec{m})$ and

$$\left[\binom{m_1}{k_1} \cdots \binom{m_\ell}{k_\ell} \right]_{\vec{k}}$$

k-particle states in each m-particle state, there will appear

$$\left[\binom{N_1}{m_1} \cdots \binom{N_\ell}{m_\ell} \right] \left[\binom{m_1}{k_1} \cdots \binom{m_\ell}{k_\ell} \right]_{\vec{k}}$$

k-particle states in the double sum. With

$$\left[\binom{N_1}{k_1} \cdots \binom{N_\ell}{k_\ell} \right]_{\vec{k}}$$

unique k-particle states in $S(\vec{k})$, we find the multiple occurrence $R_{\vec{k}}$ of each such k-particle state to be

$$R_{\vec{k}} = \frac{\left[\binom{N_1}{m_1}\cdots\binom{N_\ell}{m_\ell}\right]\left[\binom{N_1}{k_1}\cdots\binom{N_\ell}{k_\ell}\right]_{\vec{k}}}{\left[\binom{N_1-k_1}{m_1-k_1}\cdots\binom{N_\ell-k_\ell}{m_\ell-k_\ell}\right]_{\vec{k}}}$$

$$= \left[\binom{N_1-k_1}{m_1-k_1}\cdots\binom{N-k}{m-k}\right]_{\vec{k}} \quad .$$

Now, that double sum in Eq. (C.13) can be replaced by a single sum over all k-particle states in $S(\vec{k})$, with the factor of $R_{\vec{k}}$, so that we can write Eq. (C.13) as

$$\langle\langle O(k)\rangle\rangle_{S'(\vec{m})} = \sum_{\vec{k}}\left[\binom{N_1-k_1}{m_1-k_1}\cdots\binom{N_\ell-k_\ell}{m_\ell-k_\ell}\right]_{\vec{k}} \langle\langle O(k)\rangle\rangle_{S(\vec{k})} \quad , \qquad \text{(C.16a)}$$

where we have defined the trace over k-particle states in $S(\vec{k})$ as

$$\langle\langle O(k)\rangle\rangle_{S(\vec{k})} = \sum_{\Lambda\varepsilon S(\vec{k})} \sum_{\substack{\alpha,\ldots,\delta \\ \mu,\ldots,\omega}} O^{\mu,\ldots,\omega}_{\alpha,\ldots,\delta} \langle\Gamma|a_\alpha\ldots a_\delta b_\mu\ldots b_\omega|\Lambda\rangle \quad . \qquad \text{(C.16b)}$$

We can apply Wick's theorem to the diagonal k-body matrix element in Eq. (C.16b) in the same way we did to the scalar k-body trace in Eq. (C.7b). Then, after summing over the contracted labels, we can write the configuration k-body trace as

$$\langle\langle O(k)\rangle\rangle_{S(\vec{k})} = \sum_{(i,,,,j)\varepsilon S(\vec{k})} PP'(-1)^p(-1)^{p'} O^{j,\ldots,i}_{j,\ldots,i} \quad , \qquad \text{(C.16c)}$$

where P, P', p, and p' are defined in Eq. (C.7c).

If the coefficients $O^{\omega,\ldots,\delta}_{\alpha,\ldots,\delta}$ are <u>antisymmetric</u> under exchange of adjacent subscripts and under exchange of adjacent superscripts then

each of the $k!^2$ terms, that are generated by the permutation operators in Eq. (C.16c), will be equal to $O^{i,\ldots,j}_{i,\ldots,j}$. So, we can write the configuration k-particle trace as

$$\ll O(k) \gg_{S(\vec{k})} = k!^2 \sum_{(i,\ldots,j)\in S(\vec{k})} O^{i,\ldots,j}_{i,\ldots,j} \quad . \tag{C.17}$$

Since the antisymmetric coefficient $O^{i,\ldots,j}_{i,\ldots,j}$, in Eq. (C.17), will be symmetric under exchange of any pair of double labels, yet it will be zero if any pair of double labels is equal, we can unrestrict the sum over the first k_1 labels over the N_1 orbitals in the first partition, in Eq. (C.17), and likewise for the same over the labels in the other partitions. This partially restricted sum must then be divided by $(k_1!, k_2!, \ldots, k_\ell!)_{\vec{k}}$ which is the number of redundant terms. Thus, for antisymmetric coefficients, we can write the configuration k-body trace as

$$\ll O(k) \gg_{S(\vec{k})} = \frac{k!^2}{(k_1{}^i!, k_2{}^i!, \ldots, k_\ell{}^i!)_{\vec{k}}} \sum_{[i,\ldots,j]_{\vec{k}}} O^{i,\ldots,j}_{i,\ldots,j} \quad , \tag{C.18}$$

where $[i,\ldots,j]_{\vec{k}}$ denotes the partially restricted sum.

For the first example, we will find the configuration trace of a one-body operator O(1) where the configuration $\vec{m}$ contains m_1 particles in the first partition and m_2 in the second one. For k = 1, the possible configurations are $\vec{k}_1 = (1,0)$ and $\vec{k}_2 = (0,1)$. The configuration trace equation (C.16a), where the sum is now taken over configurations $\vec{k}_1$ and $\vec{k}_2$, is written as

$$\langle\langle O(1)\rangle\rangle_{S(m_1,m_2)} = \binom{N_1-1}{m_1-1}\binom{N_2}{m_2}\langle\langle O(1)\rangle\rangle_{S(\vec{k}_1)} + \binom{N_1}{m_1}\binom{N_2-1}{m_2-1}\langle\langle O(1)\rangle\rangle_{S(\vec{k}_2)} \quad .$$

Upon applying Eq. (C.18), the configuration k-body traces can then be written as

$$\langle\langle O(k)\rangle\rangle_{S(\vec{k}_1)} = \frac{1!^2}{1!\ 0!} \sum_{\alpha_1} O_{\alpha_1\alpha_1}$$

and

$$\langle\langle O(k)\rangle\rangle_{S(\vec{k}_2)} = \frac{1!^2}{0!\ 1!} \sum_{\alpha_2} O_{\alpha_2\alpha_2} \quad ,$$

where the subscript i on the single-particle state label α_i denotes a sum over all single-particle states in the i-th partition.

Next, we will find the configuration trace of a two-body operator O(2) where, again, the configuration $\vec{m}$ has two partitions. For k = 2, there are three configurations $\vec{k}$ which are defined as $\vec{k}_1 = (2,0)$, $\vec{k}_2 = (1,1)$ and $\vec{k}_3 = (0,2)$. Again, we can apply Eq. (C.16a) to this case, writing the configuration trace of the operator O(2) as

$$\langle\langle O(2)\rangle\rangle_{S(m_1,m_2)} = \binom{N_1-2}{m_1-2}\binom{N_2}{m_2}\langle\langle O(2)\rangle\rangle_{S(\vec{k}_1)} + \binom{N_1-1}{m_1-1}\binom{N_2-1}{m_2-1}\langle\langle O(2)\rangle\rangle_{S(\vec{k}_2)}$$

$$+ \binom{N_1}{m_1}\binom{N_2-2}{m_2-2}\langle\langle O(2)\rangle\rangle_{S(\vec{k}_3)} \quad .$$

Since the coefficients of this operator are antisymmetric, we can use Eq. (C.18) to write the configuration k-body traces as

$$\langle\langle O(2)\rangle\rangle_{S(\vec{k}_1)} = \frac{2!^2}{2!\ 0!} \sum_{\alpha_1\beta_1} O_{\alpha_1\beta_1\beta_1\alpha_1} \quad ,$$

$$\langle\langle O(2)\rangle\rangle_{S(\vec{k}_2)} = \frac{2!^2}{1!\ 1!} \sum_{\alpha_1\beta_2} O_{\alpha_1\beta_2\beta_2\alpha_1} \quad ,$$

and

$$\langle\langle O(2)\rangle\rangle_{S(\vec{k}_3)} = \frac{2!^2}{2!\ 0!} \sum_{\alpha_2\beta_2} O_{\alpha_2\beta_2\beta_2\alpha_2} \quad .$$

IX. APPENDIX D: ORTHOGONAL POLYNOMIALS

The topic of orthogonal polynomials, both for continuous and discrete distributions, is well-covered in many texts on mathematical statistics and numerical analysis (32,33), but we will briefly review some of their basic properties.

For a continuous weight function $\rho(x)$, which is defined over the interval L, with the property that

$$\int_L \rho(x)\, dx = 1 \quad , \tag{D.1}$$

we can define an infinite set of polynomials $P_N(x)$, where

$$P_N(x) = A_N^N x^N + A_{N-1}^N x^{N-1} + \ldots + A_0^N x^0 \tag{D.2}$$

and, which all obey the relationship

$$\int_L P_N(x)\, P_M(x)\, \rho(x)\, dx = \delta_{NM} \quad . \tag{D.3}$$

This set of polynomials will be unique if we stipulate that for each polynomial $P_N(x)$ the coefficient of the largest power of x, which is A_N^N, be greater than zero.

The coefficients of these polynomials can be solved for in ascending order of the polynomials, starting with $P_0(x)$, by applying Eq. (D.3). In doing this process, we find that first two polynomials are

$$P_0(x) = 1 \quad ,$$

and

$$P_1(x) = \frac{x - M^1}{(M^2 - (M^1)^2)^{1/2}} \quad , \tag{D.4}$$

where

$$M^N = \int_L x^n \rho(x)\, dx \quad , \quad N = 0, 1, \ldots, \infty \tag{D.5}$$

is the N-th moment of the weight function $\rho(x)$. In general, the polynomial $P_N(x)$ will be determined in terms of the first 2N moments.

On the interval L, the orthogonal polynomials $\{P_N(x)\}$ form a complete set, so that an arbitrary function $f(x)$ can be expanded as

$$f(x) = \sum_{N=0}^{\infty} C_N P_N(x) \quad . \tag{D.6}$$

If we are dealing with a <u>discrete</u> distribution of values $\{x_A: A=1, \ldots, d\}$, which can be broken up into q subsets, where the values in each subset are the same, then we can define a finite set of q polynomials $\{P_N(x): N = 0, q-1\}$ which all obey the relationship

$$\sum_{A=1}^{d} P_N(x_A) P_M(x_A) = \delta_{NM} \quad . \tag{D.7}$$

It is possible to show (33) that no polynomials exist which are of degree higher than q-1 and also obey Eq. (D.7).

We can solve for the discrete distribution polynomials in the same way we would the continuous distribution polynomials, except that we would now apply Eq. (D.7). All q polynomials will have the same form as the first q polynomials for a continuous distribution, except that

$$M^n = \sum_{A=1}^{d} (x_A)^n \quad , \quad n = 0, 1, \ldots, q-1 \quad . \qquad (D.8)$$

Note that if a continuous distribution and a discrete distribution have the same first 2q moments, that is

$$\int_L x^n \rho(x)\, dx = \sum_{A=1}^{d} (x_A)^n \quad , \quad n = 0, 1, \ldots, 2q-1 \quad , \qquad (D.9)$$

then the first q orthogonal polynomials of the continuous distribution will equal the q orthogonal polynomials of the discrete distribution, since they have the same forms with the same values for the moments.

X. APPENDIX E: MATRIX ELEMENTS OF RADIAL MOMENTS

In this appendix we will derive the one-body matrix element of the radial moment

$$\langle\alpha|r^p|\beta\rangle = \int_0^\infty R_\alpha^*(r)\, r^p\, R_\beta(r)\, dr\, \delta(j_\alpha,j_\beta)\, \delta(j_{z\alpha},j_{z\beta})\, \delta(t_{z\alpha},t_{z\beta}) \quad , \tag{E.1a}$$

where $\alpha' = (n,\ell)$, $\beta' = (n',\ell')$,

$$R_{n,\ell} = N_{n\ell}\, \exp(-\nu r^2/2)\nu_{n\ell}(r)\, r^{\ell+1} \quad , \tag{E.1b}$$

$$\nu_{n\ell}(r) = L^{\ell+1/2}_{n+\ell+1/2}(\nu r^2) = \sum_{k=0}^{n} (-1)^k\, 2^k\, \binom{n}{k}\, \frac{(2\ell+1)!!}{(2\ell+2k+1)!!}\, (\nu r^2)^k \quad , \tag{E.1c}$$

$$N^2_{n\ell} = \frac{2^{\ell-n+2}\, (2\ell+2n+1)!!\, \nu^{\ell+3/2}}{\sqrt{\pi}\, n!\, [(2\ell+1)!!]^2} \quad , \tag{E.1d}$$

$\nu = m\Omega/\hbar$, $\varepsilon_{n\ell} = (2n+\ell+3/2)\hbar\Omega$ is the single-particle eigenenergy of the harmonic oscillator wavefunctions (7), and m is the average nucleon mass. Writing the integral $I^p_{\alpha',\beta'}$ in Eq. (E.1a) in terms of Eqs. (E.1b) and (E.1c) we have

$$\begin{aligned} I^p_{\alpha',\beta'} = {} & (N_{\alpha'},N_{\beta'}) \sum_{k=0}^{n} \sum_{k'=0}^{n'} (-1)^k\, 2^k\, \binom{n}{k}\, \frac{(2\ell+1)!!}{(2\ell+2k+1)!!} \\ & \times (-1)^{k'}\, 2^{k'}\, \binom{n'}{k'}\, \frac{(2\ell'+1)!!}{(2\ell'+2k'+1)!!}\, (\nu^{1/2})^{-p-\ell-\ell'-3} \\ & \times \int_0^\infty (\nu^{1/2}r)^{p+2k+2k'+\ell+\ell'+2}\, \exp(-\nu r^2)\, d(\nu^{1/2}r) \quad . \end{aligned} \tag{E.2}$$

The integral in Eq. (E.2) can be shown (30) to be a representation of the gamma function, that is,

$$\int_0^\infty x^\alpha \exp(-x^2)dx = \Gamma\left(\frac{\alpha+1}{2}\right)/2 \quad ,$$

where $x = \nu^{1/2}r$ and $\alpha = p+2+2k'+\ell+\ell'+2$. Thus, the one-body matrix element $\langle\alpha|r^p|\beta\rangle$ can be expressed in a closed, analytic form.

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